

## THE LOCALLY COVARIANT DIRAC FIELD

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We describe the free Dirac field in a four-dimensional spacetime as a locally covariant quantum field theory in the sense of Brunetti, Fredenhagen and Verch, using a representation independent construction. The freedom in the geometric constructions involved can be encoded in terms of the cohomology of the category of spin spacetimes. If we restrict ourselves to the observable algebra, the cohomological obstructions vanish and the theory is unique. We establish some basic properties of the theory and discuss the class of Hadamard states, filling some technical gaps in the literature. Finally, we show that the relative Cauchy evolution yields commutators with the stress-energy-momentum tensor, as in the scalar field case.

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### 1. Introduction

Quantum field theory in curved spacetime is relevant for several purposes, such as the construction of cosmological models and to obtain a better understanding of quantum field theory in Minkowski spacetime. In order to achieve these goals in a more realistic setting, it is important to go beyond the well-studied free scalar field. In this paper, we will present a proof, already contained in [1], of the fact that the free Dirac field in a four-dimensional globally hyperbolic spacetime can be described as a locally covariant quantum field theory in the sense of [2].

Our presentation of the Dirac field is representation independent and we emphasize categorical methods throughout in order to point out an interesting problem concerning the uniqueness of the theory. The obstruction for the definition of a unique theory can be formulated in terms of the cohomology of the category of spacetimes with a spin structure, in particular its first Stiefel–Whitney class. It seems difficult to compute this class for a category, but we will show that a unique theory

can always be obtained by restriction to the observable algebras generated by even polynomials in the field, in which case the cohomological obstructions vanish.

Hadamard states can be defined in terms of a series expansion of their two-point distribution, detailing their local singularity structure. Alternatively, they can be characterized by a microlocal condition. The equivalence of these two definitions has been investigated by several authors using different techniques of proof, but in our opinion none of these arguments has been fully convincing. In our discussion, we hope to close any remaining gaps in the different proofs and establish the equivalence on firm ground.

We also compute the relative Cauchy evolution of this field and obtain commutators with the stress-energy-momentum tensor, in complete analogy with the scalar field case ([2]). For this, we use a point-splitting procedure to renormalize the stress-energy-momentum tensor. Because we only need commutators with this tensor we do not need to treat the so-called trace anomaly, a finite multiple of the identity operator, in detail. We refer the interested reader to [3], who also constructs the extended algebra of Wick powers, relevant for perturbation theory. A Spin-Statistics Theorem in a generally covariant framework may be found in [4].

The contents of this paper are organized as follows. In Sec. 2, we review some of the mathematical background material that we need in order to describe the Dirac field. This includes first of all the Dirac algebra and the Spin group, followed by a categorical formulation of some of the differential geometry that we will need. In Sec. 3, we describe the classical free Dirac field, starting with the geometric and algebraic aspects in Secs. 3.1 and 3.2 and the equations of motion and their fundamental solutions in Sec. 3.3. We discuss the uniqueness of the functorial constructions and their cohomological obstructions in Sec. 3.4. We then proceed to the quantum Dirac field in Sec. 4. In Sec. 4.1, we quantize the classical Dirac field in a local and covariant way and collect some of its basic properties. Section 4.2 deals with Hadamard states and includes a discussion of the existing results concerning the equivalence of the microlocal and the series expansion definitions. For this purpose we also refer to Appendix A, which contains several relevant and useful (but expected) results in microlocal analysis. Section 4.3 contains our discussion of the relative Cauchy evolution of the free Dirac field, obtaining commutators with the stress-energy-momentum tensor, but the proof of our main result there is deferred to Appendix B, because it consists of rather involved computations. Finally we end with some conclusions.

Our presentation of locally covariant quantum field theory is based on the original [2] and on [5]. For the Dirac field in curved spacetime, we largely follow [6, 7], as well as our earlier [1]. For results on Clifford algebras, we refer to [8] (see also [9] for a short review).

## 2. Mathematical Preliminaries

To prepare for our discussion of the locally covariant Dirac field, we present in the current section some mathematical preliminaries concerning the Dirac algebra, the

Spin group and a categorical formulation of relevant aspects of differential geometry. These merely serve to fix our notation and set the scene for the subsequent sections. We also point out the relations with some other definitions and conventions in the literature.

### 2.1. The Dirac algebra and the Spin group

The Spin group can be embedded in the Clifford algebra of Minkowski spacetime, which we call the Dirac algebra. Therefore, we will first briefly recall some results on Clifford algebras, for which we refer to [8] (note the difference in sign convention in the Clifford multiplication).

Let  $\mathbb{R}^{r,s}$  be a finite dimensional real vector space with dimension  $n = r + s$  and with a non-degenerate bilinear form  $g_{ab}$  which has  $r$  positive and  $s$  negative eigenvalues. The Clifford algebra  $Cl_{r,s}$  is defined as the  $\mathbb{R}$ -linear associative algebra generated by a unit element  $I$  and an orthonormal basis  $e_a$  of  $\mathbb{R}^{r,n-r}$  subject to the relations:

$$e_a e_b + e_b e_a = 2g_{ab} I.$$

This definition is independent of the choice of basis. We may identify  $\mathbb{R}^{r,s} \subset Cl_{r,s}$  as the subspace of monomials in the basis  $e_a$  of degree one. The even, respectively odd, subspace of this Clifford algebra is the one spanned by monomials of even, respectively odd, degree in the basis vectors and is denoted by  $Cl_{r,s}^0$ , respectively  $Cl_{r,s}^1$ . Note that the even subspace is also a subalgebra. In the following we will be especially interested in Minkowski spacetime,  $M_0 := \mathbb{R}^{1,3}$ , where the bilinear form is  $\eta = \text{diag}(1, -1, -1, -1)$  and where we choose an orthonormal basis  $g_a$ ,  $a = 0, 1, 2, 3$  with  $\|g_0\|^2 = 1$ ,  $\|\cdot\|^2$  denoting the Minkowski pseudo-norm squared. The associated Clifford algebra is called the Dirac algebra  $D := Cl_{1,3}$  and it is characterized by

$$g_a g_b + g_b g_a = 2\eta_{ab} I. \quad (1)$$

As a vector space, the Clifford algebra is naturally isomorphic to the exterior algebra. This motivates the term *volume form* for the element  $g_5 := g_0 g_1 g_2 g_3$  (or in general  $e := e_1 \cdots e_{r+s}$ ). Note the following properties:

**Lemma 2.1.** *We have  $g_5^2 = -I$  and  $g_5 v g_5^{-1} = -v$  for all  $v \in M_0$ . More generally, if  $u \in M_0$  has  $u^2 = \|u\|^2 I \neq 0$ , then  $u^{-1} = \frac{1}{\|u\|^2} u$  and  $v \mapsto -uvu^{-1}$  defines a reflection of  $M_0$  in the hyperplane perpendicular to  $u$ .*

**Proof.** These equalities follow directly from Eq. (1). For the last claim, e.g., we compute:

$$-uvu^{-1} = v - (uv + vu)u^{-1} = v - \frac{2\langle u, v \rangle}{\|u\|^2} u, \quad v \in M_0. \quad \square$$

Standard arguments with Clifford algebras [8] give:

$$D = Cl_{1,3} \simeq Cl_{1,4}^0 \simeq Cl_{4,1}^0, \quad Cl_{4,1} \simeq M(4, \mathbb{C}),$$

where  $M(4, \mathbb{C})$  denotes the algebra of complex  $(4 \times 4)$ -matrices. In fact,  $Cl_{4,1}$  is generated by the generators  $g_a$  of  $D$  together with a central element  $\omega$ , corresponding to  $iI \in M(4, \mathbb{C})$ . Hence:

$$M(4, \mathbb{C}) \simeq \mathbb{C} \otimes_{\mathbb{R}} D. \quad (2)$$

This also implies that the center of  $D$  is spanned by  $I$  (over  $\mathbb{R}$ ). The following Fundamental Theorem provides all the essential information we need on the Dirac algebra (for an elementary algebraic proof, we refer to Pauli [10].):

**Theorem 2.2 (Fundamental Theorem).** *The Dirac algebra  $D$  is simple and has a unique irreducible complex representation (i.e. an  $\mathbb{R}$ -linear representation  $\pi: D \rightarrow M(n, \mathbb{C})$ ), up to equivalence. This is the representation  $\pi_0: D \rightarrow M(4, \mathbb{C})$  determined by  $\pi_0(g_a) = \gamma_a$  with the Dirac matrices*

$$\gamma_0 := \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \gamma_i := \begin{pmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{pmatrix},$$

where  $\sigma_i$  are the Pauli matrices  $\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ,  $\sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$  and  $\sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ . The equivalence with another irreducible complex representation  $\pi$  of  $D$  is implemented by  $\pi(S) = L\pi_0(S)L^{-1}$  for all  $S \in D$ , where  $L \in GL(4, \mathbb{C})$  is unique up to a non-zero complex factor.

Consequently, for every set of matrices  $\gamma'_a \in M(4, \mathbb{C})$  satisfying Eq. (1) there is an  $L \in GL(4, \mathbb{C})$ , unique up to a non-zero complex constant, such that  $\gamma'_a = L\gamma_a L^{-1}$ .

**Proof.** One can show [8] that  $D \simeq M(2, \mathbb{H})$ , where  $\mathbb{H}$  is the skew field of quaternions. This algebra is simple, because it is a full matrix algebra. The given matrices  $\gamma_a$  satisfy the Clifford relations (1) and therefore extend to a representation of  $D$  in  $M(4, \mathbb{C})$ .

Any complex representation  $\pi: D \rightarrow M(n, \mathbb{C})$  extends to a complex representation  $\tilde{\pi}$  of  $M(4, \mathbb{C})$ , using Eq. (2) and the trivial center of  $D$ , which is irreducible if  $\pi$  is irreducible. As  $M(4, \mathbb{C})$  has only one irreducible representation up to equivalence (see [11]), namely the defining one on  $\mathbb{C}^4$ , this determines  $\pi$  up to equivalence, as stated. If  $K, L \in GL(4, \mathbb{C})$  are two matrices which implement the same equivalence, then  $KL^{-1}$  commutes with  $D$  and hence  $K = cL$ , where  $c \in \mathbb{C}$  is non-zero because  $K$  is invertible. Note that  $\pi'(g_a) := \gamma'_a$  extends to a complex representation of  $D$  in  $M(4, \mathbb{C})$  which is faithful (as  $D$  is simple). The last statement then follows from the previous one.  $\square$

For notational convenience, we define  $\gamma_5 := \pi_0(g_5)$ .

We can define a determinant and trace function on  $D$  by  $\det S = \det \pi(S)$  and  $\text{Tr}(S) = \text{Tr}(\pi(S))$  for all  $S \in D$ , where  $\pi$  is any irreducible complex representation of  $D$ . This is well-defined by the Fundamental Theorem. The following lemma is often useful in computations:

**Lemma 2.3.** *We have  $\text{Tr}(g_a g_b) = 4\eta_{ab}$  and  $\text{Tr}([g_b, g_c]g_d g_a) = 8(\eta_{cd}\eta_{ba} - \eta_{bd}\eta_{ca})$ .*

**Proof.** Using the cyclicity of the trace and Eq. (1) we find:  $\text{Tr}(g_a g_b) = \frac{1}{2} \text{Tr}(g_a g_b + g_b g_a) = \text{Tr}(\eta_{ab} I) = 4\eta_{ab}$  and

$$\begin{aligned} \text{Tr}([g_b, g_c] g_d g_a) &= \text{Tr}(g_b [g_c, g_d g_a]) = \text{Tr}(g_b \{g_c, g_d\} g_a - g_b g_d \{g_c, g_a\}) \\ &= 2 \text{Tr}(\eta_{cd} g_b g_a - g_b g_d \eta_{ca}) = 8(\eta_{cd} \eta_{ba} - \eta_{bd} \eta_{ca}). \end{aligned}$$

□

We now turn to the Spin group, which is the universal covering group of the special Lorentz group, a double covering which can be constructed in an elegant way inside the Dirac algebra.

**Definition 2.4.** The Pin and Spin groups of  $Cl_{r,s}$  are defined as

$$\begin{aligned} Pin_{r,s} &:= \{S \in Cl_{r,s} \mid S = u_1 \cdots u_k, u_i \in \mathbb{R}^{r,s}, u_i^2 = \pm I\}, \\ Spin_{r,s} &:= Pin_{r,s} \cap Cl_{r,s}^0. \end{aligned}$$

We let  $Spin_{1,3}^0$  denote the connected component of  $Spin_{1,3}$  which contains the identity.

We also define the Lorentz group  $\mathcal{L} := O_{1,3}$ , the special Lorentz group  $\mathcal{L}_+ := SO_{1,3}$  and the special orthochronous Lorentz group  $\mathcal{L}_+^\uparrow := SO_{1,3}^0$ , which is the connected component of  $\mathcal{L}_+$  containing the identity.

The special orthochronous Lorentz group preserves the orientation and time-orientation. For  $S \in Pin_{1,3}$  the map  $v \mapsto SvS^{-1}$  on  $M_0$  is a product of reflections (up to a sign) by Lemma 2.1. Together with the fact that  $\det u = \|u\|^4$  for all  $u \in M_0$  this gives rise to another useful characterisation of the group  $Pin_{1,3}$ , which we shall not prove<sup>a</sup>:

**Proposition 2.5.**  $Pin_{1,3} = \{S \in D \mid \det S = 1, \forall v \in M_0 SvS^{-1} \in M_0\}$ .

It can be seen from Proposition 2.5 that  $Pin_{1,3}$  and  $Spin_{1,3}$  are indeed Lie groups. For the universal covering homomorphism  $\Lambda$  between  $Pin_{1,3}$  and the Lorentz group, we have the following formulae<sup>b,c</sup>:

**Proposition 2.6.** *The map  $\Lambda: Pin_{1,3} \rightarrow \mathcal{L}$  defined by  $S \mapsto \Lambda_b^a(S) \in M(4, \mathbb{R})$  such that  $Sg_b S^{-1} = g_a \Lambda_b^a(S)$  is the universal covering homomorphism of Lie groups, which restricts to the universal covering homomorphism  $Spin_{1,3}^0 \rightarrow \mathcal{L}_+^\uparrow$ . We have  $\Lambda_b^a(S) = \frac{1}{4} \text{Tr}(g^a Sg_b S^{-1})$  and the inverse of the derivative  $d\Lambda: spin_{1,3}^0 \rightarrow l_+^\uparrow$  at*

<sup>a</sup>The definition of the Spin group in [12] corresponds to our group  $Pin_{1,3}$ . In [6, 7] one uses the term Spin group for the group

$$\mathcal{S} := \{S \in M(4, \mathbb{C}) \mid \det S = 1, SvS^{-1} \in M_0 \text{ for all } v \in M_0\}.$$

Note that this group cannot give a double covering of the Lorentz group, as claimed in [6] (but not in [7]), because for any  $S \in \mathcal{S}$  the matrices  $iS, -S, -iS$  are in  $\mathcal{S}$  too. Its usefulness is based on its simple definition and the fact that  $\mathcal{S}^0 = Spin_{1,3}^0$ .

<sup>b</sup>These results are well known, but we record them for definiteness to correct a sign error in the spin connection (5) that has occurred in [6, 7, 13].

<sup>c</sup>Lower case Latin indices are raised and lowered with  $\eta^{ab}$ , respectively,  $\eta_{ab}$  throughout.

$S = I$  is given by:

$$(d\Lambda)^{-1}(\lambda^b_a) = \frac{1}{4}\lambda^b_a g_b g^a.$$

**Proof.** For the first sentence we refer to [8, Theorem 2.10] and subsequent remarks. Using the Clifford relations (1), we see that

$$\begin{aligned}\Lambda^a_b(S) &= \frac{1}{4}\eta^{ac}\mathrm{Tr}(\eta_{cd}\Lambda^d_b(S)I) = \frac{1}{8}\eta^{ac}\mathrm{Tr}((g_c g_d + g_d g_c)\Lambda^d_b(S)) \\ &= \frac{1}{4}\eta^{ac}\mathrm{Tr}(g_c g_d \Lambda^d_b(S)) = \frac{1}{4}\mathrm{Tr}(g^a S g_b S^{-1}).\end{aligned}$$

Expanding  $\Lambda(S + \epsilon s + O(\epsilon^2))$  up to second order in  $\epsilon$  we find  $d\Lambda(s)^a_b = \frac{1}{4}\mathrm{Tr}([g_b, g^a]s)$ . We check that  $L(\lambda^b_a) := \frac{1}{4}\lambda^b_a g_b g^a$  is an inverse of  $d\Lambda$ :

$$\begin{aligned}d\Lambda(L(\lambda^d_e))^a_b &= \frac{1}{16}\eta^{ac}\eta^{ef}\lambda^d_e\mathrm{Tr}([g_b, g_c]g_d g_f) = \frac{1}{2}\eta^{ac}\eta^{ef}\lambda^d_e(\eta_{cd}\eta_{bf} - \eta_{bd}\eta_{cf}) \\ &= \frac{1}{2}(\lambda^a_b - \eta^{ae}\eta_{bd}\lambda^d_e) = \lambda^a_b,\end{aligned}$$

where we used Lemma 2.3 and the symmetry properties of  $\lambda^d_e \in l^\uparrow_+$  in the last line.  $\square$

## 2.2. Some category theory and differential geometry

The language of locally covariant quantum field theory uses category theory to express the physical ideas of locality and covariance. Any object or construction that is extended from a single spacetime (usually Minkowski spacetime) to the categorical framework gets the adjective “locally covariant”. The essence of local covariance seems to have a geometric origin and, because the Dirac field in curved spacetimes involves a substantial amount of geometric constructions, it will be convenient to present the relevant differential geometry in a categorical setting here. We refrain from the urge to call this “locally covariant differential geometry”, which appears to be a pleonasm.

A *category*  $\mathfrak{C}$  consists of a set of objects  $c$  and a set of morphisms or arrows<sup>d</sup>  $\gamma: c_1 \rightarrow c_2$  between objects of  $\mathfrak{C}$ , such that the composition of morphisms, when defined, is associative and each object admits an identity morphism (we refer to [14] for more details). A (*covariant*) *functor*  $\mathbf{F}: \mathfrak{C} \rightarrow \mathfrak{B}$  is a map between categories, which maps objects  $c$  to objects  $\mathbf{F}(c)$  and morphisms  $\gamma: c_1 \rightarrow c_2$  to morphisms  $\mathbf{F}(\gamma): \mathbf{F}(c_1) \rightarrow \mathbf{F}(c_2)$  such that an identity morphism maps to an identity morphism and the composition of morphisms is preserved. A *contravariant functor*  $\mathbf{F}: \mathfrak{C} \rightarrow \mathfrak{B}$  is defined similarly, but reverses the direction of the morphisms:  $\mathbf{F}(\gamma): \mathbf{F}(c_2) \rightarrow \mathbf{F}(c_1)$ . A *natural transformation*  $t: \mathbf{F} \Rightarrow \mathbf{G}$  between covariant functors  $\mathbf{F}: \mathfrak{C} \rightarrow \mathfrak{B}$  and  $\mathbf{G}: \mathfrak{C} \rightarrow \mathfrak{B}$  is a map which assigns to each object  $c$  a morphism  $t(c)$  of  $\mathfrak{B}$ , called the *component* of  $t$  at  $c$ , such that for every morphism  $\gamma: c_1 \rightarrow c_2$

<sup>d</sup>It is very often convenient to depict the morphisms in a diagram as arrows between objects.

of  $\mathfrak{C}$  we have  $t(c_2) \circ \mathbf{F}(\gamma) = \mathbf{G}(\gamma) \circ t(c_1)$ , which can be depicted as a commutative diagram. When a natural transformation  $t$  admits another natural transformation  $s$  such that  $t(c) \circ s(c) = \text{id}_c = s(c) \circ t(c)$  for all objects  $c$ , then  $t$  is called a *natural equivalence*. In this case, we write  $t: \mathbf{F} \Leftrightarrow \mathbf{G}$ . A natural transformation between contravariant functors or between a covariant and a contravariant functor is defined similarly, except that some arrows in the commutative diagram are reversed.

A subcategory  $\mathfrak{B}$  of  $\mathfrak{C}$  consists of a subset of the objects of  $\mathfrak{C}$  and a subset of its morphisms in such a way that  $\mathfrak{B}$  still satisfies the axioms of a category. In our case, all categories will be concrete, i.e. the objects will be sets with a certain structure and the morphisms will be maps between sets. The identity morphism will always be the identity map and the composition of maps, when defined, is automatically associative. In short, our categories will be subcategories of the category  $\mathfrak{Set}$ , whose objects are sets<sup>e</sup> and whose morphisms are maps.

For our discussion of differential geometry we start with the following

**Definition 2.7.** The category  $\mathfrak{Man}^n$  of smooth manifolds is the category whose objects are  $C^\infty$  manifolds  $\mathcal{M}$  of (finite) dimension  $n$  and whose morphisms are  $C^\infty$  embeddings  $\mu: \mathcal{M}_1 \rightarrow \mathcal{M}_2$ .

The category  $\mathfrak{Bund}'$  of fiber bundles is the category whose objects are smooth fiber bundles  $p: \mathcal{B} \rightarrow \mathcal{M}$  over objects  $\mathcal{M}$  of  $\mathfrak{Man}^n$  with bundle projection map  $p$ , and whose morphisms are  $C^\infty$  maps  $\beta: \mathcal{B}_1 \rightarrow \mathcal{B}_2$  covering a morphism  $\mu: \mathcal{M}_1 \rightarrow \mathcal{M}_2$  of  $\mathfrak{Man}^n$ , i.e. such that  $p_2 \circ \beta = \mu \circ p_1$ . We denote by  $\mathfrak{Bund}$  the subcategory whose morphisms restrict to isomorphisms of the fibers.

The categories  $\mathfrak{VBund}'_{\mathbb{R}}$ , respectively  $\mathfrak{VBund}'_{\mathbb{C}}$ , of real (complex) vector bundles is the subcategory of  $\mathfrak{Bund}'$  whose objects  $\mathcal{V}$  are real (complex) vector bundles and whose morphisms  $\nu: \mathcal{V}_1 \rightarrow \mathcal{V}_2$  are real (complex) linear maps of the fibers. Again we denote by  $\mathfrak{VBund}_{\mathbb{R}}$  and  $\mathfrak{VBund}_{\mathbb{C}}$  the subcategories whose morphisms restrict to isomorphisms of the fibers.

We could have taken all smooth maps between manifolds as morphisms of  $\mathfrak{Man}^n$  or allowed all dimensions. However, local diffeomorphisms allow us to transport more structure, which enables us to describe more of the canonical differential geometric constructions as functors. We describe the most important examples below. For fiber bundles, on the other hand, it will be useful to allow maps which are not isomorphisms on the fibers.<sup>f,g</sup>

<sup>e</sup>See [14] for some relevant remarks concerning the foundations of set theory and the use of small sets.

<sup>f</sup>The unprimed categories, whose morphisms are isomorphisms of the fibers, can be described as fibered categories over  $\mathfrak{Man}^n$ , cf. [15, p. 44].

<sup>g</sup>The functors  $\mathbf{B}: \mathfrak{Man}^n \rightarrow \mathfrak{Bund}'$  below are all of a special type, namely, they associate to a manifold  $\mathcal{M}$  a fiber bundle whose base space is again  $\mathcal{M}$ . Although we will only use functors of this type when describing the Dirac field, the restriction is not technically necessary in our definitions.

Two of the most basic functors in differential geometry are

The **tangent bundle** functor  $\mathbf{T}:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  assigns to every manifold  $\mathcal{M}$  the tangent bundle  $T\mathcal{M}$  and to every morphism  $\mu:\mathcal{M}_1 \rightarrow \mathcal{M}_2$  the differential  $d\mu:T\mathcal{M}_1 \rightarrow T\mathcal{M}_2$ .

The **cotangent bundle** functor<sup>h</sup>  $\mathbf{T}^*:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  assigns to every manifold  $\mathcal{M}$  the cotangent bundle  $T^*\mathcal{M}$  and to every morphism  $\mu:\mathcal{M}_1 \rightarrow \mathcal{M}_2$  the push-forward  $\mu_*:T\mathcal{M}_1 \rightarrow T\mathcal{M}_2$ , which is defined as  $\mu_*\omega := \omega \circ d\mu^{-1}$ .

In a similar way, one can define the functor  $\Lambda^k:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  of exterior  $k$ -forms and the exterior algebra functor  $\Lambda:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$ , both with push-forwards. Another example is

The **density bundle** functor  $|\Lambda^n|:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  assigns to every spacetime  $\mathcal{M}$  the one-dimensional trivial vector bundle of densities  $|\Lambda^n\mathcal{M}|$ , where  $n$  is the dimension of  $\mathcal{M}$ . This is the vector bundle whose fiber at  $x \in \mathcal{M}$  consists of functions  $d:\Lambda_x^n\mathcal{M} \rightarrow \mathbb{R}$  such that  $d(r\omega) = |r|\omega$  for all  $r \in \mathbb{R}$  and  $\omega \in \Lambda_x^n\mathcal{M}$  (cf. [16, Appendix A.3]). A morphism  $\mu$  is mapped to the push-forward defined by  $\mu_*d := d \circ \mu^*$ , where  $\mu^*\omega := \omega \circ d\mu$  is the pull-back.

By standard constructions, one can take (finite) direct sums and tensor products of functors from  $\mathcal{M}\mathbf{an}^n$  into  $\mathfrak{VBund}'_{\mathbb{R}}$  which map  $\mathcal{M}$  into a vector bundle over  $\mathcal{M}$ . One obtains another such functor in the obvious way. For functors  $\mathbf{V}$  into  $\mathfrak{VBund}_{\mathbb{R}}$  one can also define the dual, denoted by  $\mathbf{V}^*$ , where the morphism between dual vector bundles is the push-forward of the original morphism. This generalizes the example of  $\mathbf{T}^*$  above. As another standard construction one can define the complexification  $\mathbf{V}_{\mathbb{C}}$  of any functor  $\mathbf{V}$  into  $\mathfrak{VBund}'_{\mathbb{R}}$  (respectively,  $\mathfrak{VBund}_{\mathbb{R}}$ ), which is a functor into  $\mathfrak{VBund}'_{\mathbb{C}}$  (respectively,  $\mathfrak{VBund}_{\mathbb{C}}$ ).

Now we turn to some examples of natural transformations:

The **canonical pairing** between a functor  $\mathbf{V}:\mathcal{M}\mathbf{an}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  which maps  $\mathcal{M}$  to a vector bundle  $V\mathcal{M}$  over  $\mathcal{M}$  and its dual  $\mathbf{V}^*$  is a natural transformation  $\langle \cdot, \cdot \rangle:\mathbf{V}^* \otimes \mathbf{V} \Rightarrow \Lambda^0$  whose components cover the identity morphism.

**Complex conjugation** is a natural equivalence  $\bar{\cdot}:\mathbf{V}_{\mathbb{C}} \Leftrightarrow \mathbf{V}_{\mathbb{C}}$  in  $\mathfrak{VBund}_{\mathbb{R}}$  (or  $\mathfrak{VBund}'_{\mathbb{R}}$ ) between complexified vector bundles, which sends each section to its complex conjugate.

A further example of a natural equivalence is the fiber-wise multiplication by a real number  $r \neq 0$ . (For  $r = 0$ , this only yields a natural transformation.) Furthermore, the constructions mentioned above (dual, direct sum, tensor product) and the natural transformations (pairing, fiber-wise multiplication) can also be applied directly to complex vector bundles in a canonical (Hermitean) way.

<sup>h</sup>It is tempting to think of a *contravariant* functor that maps manifolds to their cotangent bundles and morphisms  $\mu$  to the pull-back,  $\mu^*\omega := \omega \circ d\mu$ , which indeed reverses the directions of arrows and changes the order of compositions. However, the pull-back is only defined on the image of  $\mu$ , so in general this does not define a morphism in  $\mathfrak{VBund}'_{\mathbb{R}}$ .



It will be convenient to consider distributions and integration in a categorical setting too:

**Definition 2.8.**  $\mathfrak{TVec}$  is the category of topological vector spaces with injective continuous linear maps as morphisms. The functor  $\mathbb{C}:\mathfrak{Man}^n \rightarrow \mathfrak{TVec}$  is the constant functor  $\mathbb{C}$ , i.e. it assigns to each object the one dimensional space  $\mathbb{C}$  and to each morphism the identity morphism.

The *functor of test-sections* is the functor  $\mathbf{C}_0^\infty:\mathfrak{VBund}'_{\mathbb{C}} \rightarrow \mathfrak{TVec}$  which maps each complex vector bundle  $\mathcal{V}$  to the space  $C_0^\infty(\mathcal{V})$  of compactly supported smooth sections of  $\mathcal{V}$  in the test-section topology.<sup>i</sup> A morphism  $\nu$ , covering a morphism  $\mu$ , is mapped to the push-forward  $\nu_*$  defined by  $\nu_*(f) = \nu \circ f \circ \mu^{-1}$  on  $\mu(\mathcal{M}_1)$ , extended by 0 to all of  $\mathcal{M}_2$ .

The *functor of smooth sections* is the contravariant functor  $\mathbf{C}^\infty:\mathfrak{VBund}_{\mathbb{C}} \rightarrow \mathfrak{TVec}$  which maps each complex vector bundle  $\mathcal{V}$  to the space  $C^\infty(\mathcal{V})$  of smooth sections of  $\mathcal{V}$  in the usual topology. A morphism  $\nu$ , covering a morphism  $\mu$ , is mapped to the pull-back  $\nu^*$  defined by  $\nu^*(f) = \nu^{-1} \circ f \circ \mu$ .

The *functor of distributions* is the contravariant functor  $\mathbf{Distr}:\mathfrak{VBund}'_{\mathbb{C}} \rightarrow \mathfrak{TVec}$  which maps each complex vector bundle  $\mathcal{V}$  to the space  $(C_0^\infty(\mathcal{V}))'$  of distributions on  $\mathcal{V}$  with the weak topology induced by  $C_0^\infty(\mathcal{V})$ . A morphism  $\nu$ , covering a morphism  $\mu$ , is mapped to the pull-back  $\nu^*$  defined by  $\nu^*u := u \circ \nu_*$ .

We will not need compactly supported distributions, but they can be defined as the functor dual to  $\mathbf{C}^\infty$ . Notice that objects which are not compactly supported, such as smooth sections or distributions, behave contravariantly, whereas compactly supported ones behave covariantly. Also note that the pull-back of a smooth section can only be defined for morphisms that restrict to isomorphisms of the fibers. The following constructions will be of importance in Sec. 4:

**Integration** is a natural transformation  $\int:\mathbf{C}_0^\infty \circ |\Lambda^n| \Rightarrow \mathbb{C}$  which assigns to each  $\omega \in C_0^\infty(|\Lambda^n \mathcal{M}|)$  the integral  $\int_{\mathcal{M}} \omega$ .

**Canonical Injections.** Let  $\mathbf{f}:\mathfrak{VBund}_{\mathbb{C}} \rightarrow \mathfrak{VBund}'_{\mathbb{C}}$  be the forgetful functor. For any functor  $\mathbf{V}:\mathfrak{Man}^n \rightarrow \mathfrak{VBund}_{\mathbb{C}}$  there is a canonical natural transformation  $\kappa:\mathbf{C}_0^\infty \circ \mathbf{f} \circ \mathbf{V} \Rightarrow \mathbf{C}^\infty \circ \mathbf{V}$ , whose components are the canonical injections  $C_0^\infty(V\mathcal{M}) \subset C^\infty(V\mathcal{M})$ . Similarly, there is a canonical natural transformation  $\iota:\mathbf{C}^\infty \circ (\mathbf{V} \otimes |\Lambda^n|) \Rightarrow \mathbf{Distr} \circ \mathbf{f} \circ \mathbf{V}^*$  given by  $\iota_{\mathcal{M}}(f \otimes \omega) := \int_{\mathcal{M}} \langle \cdot, f \rangle \omega$  for any smooth section  $f$  of  $V\mathcal{M}$  and any density  $\omega$  on  $\mathcal{M}$ . Each component of  $\iota$  is injective.

Where convenient we will identify a functor  $\mathbf{V}:\mathfrak{Man}^n \rightarrow \mathfrak{VBund}_{\mathbb{C}}$  with the functor  $\mathbf{f} \circ \mathbf{V}$ , omitting the forgetful functor, as this rarely leads to confusion. Furthermore, any natural transformation  $t:\mathbf{V}_1 \Rightarrow \mathbf{V}_2$  between a pair of functors  $\mathbf{V}_i:\mathfrak{Man}^n \rightarrow \mathfrak{VBund}'_{\mathbb{C}}$ ,  $i = 1, 2$ , lifts to a corresponding natural transformation

<sup>i</sup>For a precise definition of the well-known topologies on test-sections and smooth sections we refer to [17, Chap. 17].

$T: \mathbf{C}_0^\infty \circ \mathbf{V}_1 \Rightarrow \mathbf{C}_0^\infty \circ \mathbf{V}_2$  defined pointwise by  $T_{\mathcal{M}}f := t_{\mathcal{M}} \circ f$ . The same statement holds for  $T: \mathbf{C}^\infty \circ \mathbf{V}_1 \Rightarrow \mathbf{C}^\infty \circ \mathbf{V}_2$ , if the  $\mathbf{V}_i$  are functors into the category  $\mathfrak{VBund}_{\mathbb{C}}$ .

Next we add the structure of a semi-Riemannian metric:

**Definition 2.9.** The category  $\mathfrak{SRMan}^n$  of semi-Riemannian manifolds is the subcategory of  $\mathfrak{Man}^n$  whose objects  $M = (\mathcal{M}, g)$  are  $C^\infty$  manifolds  $\mathcal{M}$  of dimension  $n$  with a semi-Riemannian metric  $g$  and whose morphisms  $m: M_1 \rightarrow M_2$  are given by the isometric morphisms in  $\mathfrak{Man}^n$ , i.e. morphisms  $\mu: \mathcal{M}_1 \rightarrow \mathcal{M}_2$  such that  $\mu^*g_1 = g_2|_{\mu(\mathcal{M}_1)}$ .

Again there is a canonical forgetful functor  $\mathbf{f}: \mathfrak{SRMan}^n \rightarrow \mathfrak{Man}^n$ , which is often left implicit, so we will write e.g.  $\mathbf{T}$  for the functor  $\mathbf{T} \circ \mathbf{f}$ . The extra structure of a semi-Riemannian metric gives rise to extra functors and natural equivalences that are of interest to us:

The **metric identification** is a natural equivalence  $G: \mathbf{T} \Leftrightarrow \mathbf{T}^*$  whose component at  $M = (\mathcal{M}, g)$  is given by the map  $G_{\mathcal{M}}: T\mathcal{M} \rightarrow T^*\mathcal{M}$  such that  $v \mapsto g(v, \cdot)$ .

The **frame bundle** functor  $\mathbf{F}: \mathfrak{SRMan}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  assigns to each object  $M$  the frame bundle  $F\mathcal{M}$ , i.e. the bundle whose fiber at a point  $x \in \mathcal{M}$  consists of all orthonormal bases of  $T_x\mathcal{M}$  in the metric  $g$ . This fiber is a subset of  $T^{\otimes n}\mathcal{M}$ . A morphism  $m$  is mapped to the push-forward  $\mu_*$  acting on  $F\mathcal{M} \subset T^{\otimes n}\mathcal{M}$ .

The **volume form** functor  $\mathbf{vol}: \mathfrak{SRMan}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$  is defined as  $\mathbf{vol} := |\Lambda^n| \circ \mathbf{f}$ . When  $m: M_1 \rightarrow M_2$  is a morphism and  $d\text{vol}_i := \sqrt{|\det g_i|}$  the metric induced volume form on  $M_i$ , then  $\mathbf{vol}$  maps  $d\text{vol}_1$  to the restriction of  $d\text{vol}_2$  to  $m(\mathcal{M}_1)$ . There is a canonical natural equivalence from  $\Lambda^0$  to  $\mathbf{vol}$ , which consists of multiplication with the metric induced volume form.

Similarly there are natural equivalences between any functor  $\mathbf{V}: \mathfrak{SRMan}^n \rightarrow \mathfrak{VBund}_{\mathbb{C}}$  and  $\mathbf{V} \otimes |\Lambda^n|$ . Therefore we obtain a canonical natural transformation  $\iota: \mathbf{C}^\infty \circ \mathbf{V} \Rightarrow \mathbf{Distr} \circ \mathbf{V}^*$  whose components are injective.

Finally

we should mention the Clifford bundle functor  $\mathbf{Cl}: \mathfrak{SRMan}^n \rightarrow \mathfrak{VBund}_{\mathbb{R}}$ , which assigns to each object  $M = (\mathcal{M}, g)$  the Clifford bundle  $Cl\mathcal{M}$ , which is the vector bundle whose fiber at  $x \in \mathcal{M}$  is the Clifford algebra of  $(T_x\mathcal{M}, g)$  viewed as a linear space. Ignoring the algebraic structure, this functor is naturally equivalent to  $\Lambda \circ \mathbf{f}$ . Although we will not do so, it is possible to use this functor as a basic object for the description of fermions (cf. [18]).

### 3. The Classical Dirac Field

After these mathematical preliminaries we are now ready to start constructing the classical free Dirac field (as a locally covariant classical field). We will first describe the geometric and algebraic constructions, before we discuss the Dirac equation and its fundamental solutions. We close by investigating to what extent the relations between the Dirac operator, charge conjugation and adjoint map fix the structure

of the theory and find that the non-uniqueness can be characterised in terms of the cohomology of the category of spin spacetimes.

### 3.1. Geometric aspects

In order to describe the Dirac field we need to introduce the notion of a spin structure on a spacetime, combining the geometric and the algebraic results of Sec. 2. This is the purpose of the current subsection.

The systems that we will consider are intended to model Dirac quantum fields living in a (region of) spacetime which is endowed with a fixed Lorentzian metric (a background gravitational field). Mathematically these regions are modelled as follows:

**Definition 3.1.** By the term *globally hyperbolic spacetime* we will mean a connected, Hausdorff,  $C^\infty$  Lorentzian manifold  $M = (\mathcal{M}, g)$  of dimension  $d = 4$ , which is oriented, time-oriented and admits a Cauchy surface.

A subset  $O \subset \mathcal{M}$  of a globally hyperbolic spacetime  $M$  is called *causally convex* iff for all  $x, y \in O$  all causal curves in  $\mathcal{M}$  from  $x$  to  $y$  lie entirely in  $O$ .

The category  $\mathbf{Spac}$  is the subcategory of  $\mathbf{GRMan}^n$  whose objects are all globally hyperbolic spacetimes  $M = (\mathcal{M}, g)$  and whose morphisms are isometric embeddings  $\psi$  that preserve the orientation and time-orientation and such that  $\psi(\mathcal{M}_1)$  is causally convex.

By a theorem of Geroch any globally hyperbolic spacetime is paracompact ([19, Appendix]).

Most notations we use concerning the causal structure of spacetimes are standard, cf. [20]. The importance of causally convex sets is that for any morphism  $\psi$  the causal structure of  $M_1$  coincides with that of  $\psi(M_1)$  inside  $M_2$ :

$$\psi(J_{M_1}^\pm(x)) = J_{M_2}^\pm(\psi(x)) \cap \psi(\mathcal{M}_1), \quad x \in \mathcal{M}_1.$$

If  $O \subset \mathcal{M}$  is a connected open causally convex set, then  $(O, g|_O)$  defines a globally hyperbolic spacetime in its own right. In this case there is a canonical morphism  $I_{M,O} : O \rightarrow M$  given by the canonical embedding  $\iota : O \rightarrow \mathcal{M}$ . We will often drop  $I_{M,O}$  and  $\iota$  from the notation and simply write  $O \subset M$ .

Notice that there is a forgetful functor  $\mathbf{f} : \mathbf{Spac} \rightarrow \mathbf{GRMan}^n$  and that we can define the functor  $\mathbf{F}_+^\dagger : \mathbf{Spac} \rightarrow \mathbf{Bund}$  of oriented, time-oriented orthonormal frames  $F_+^\dagger \mathcal{M}$  for the tangent bundle, in analogy to Sec. 2.2. This is a principal  $\mathcal{L}_+^\dagger$ -bundle over  $M$ , where the special orthochronous Lorentz group  $\mathcal{L}_+^\dagger$  acts from the right, i.e., given  $e = (x, e_0, \dots, e_3) \in F_+^\dagger M$ , where  $x \in \mathcal{M}$  and  $e_a \in T_x M$  such that  $g_x(e_a, e_b) = \eta_{ab}$  and  $e_0$  is future pointing, the action of  $\Lambda$  is defined by  $R_\Lambda e = e' = (x, e'_0, \dots, e'_3)$  where  $e'_a = e_b \Lambda^b_a$ .

**Definition 3.2.** A *spin structure* on  $M$  is a pair  $(SM, \pi)$ , where  $SM$  is a principal  $Spin_{1,3}^0$ -bundle over  $M$ , the *spin frame bundle*, with a right action  $R_S$ ,  $S \in Spin_{1,3}^0$ ,

and  $\pi: SM \rightarrow FM$ , the *spin frame projection*, is a base-point preserving bundle homomorphism such that

$$\pi \circ R_S = R_{\Lambda(S)} \circ \pi,$$

where  $S \mapsto \Lambda(S)$  is the universal covering map (cf. Proposition 2.6).

A globally hyperbolic *spin spacetime*  $SM = (\mathcal{M}, g, SM, \pi)$  is an object  $M = (\mathcal{M}, g)$  of  $\mathfrak{Spac}$  which is endowed with the spin structure  $(SM, \pi)$ .

The category  $\mathfrak{S}\mathfrak{Pac}$  is the subcategory of  $\mathfrak{Bund}$  whose objects are all globally hyperbolic spin spacetimes  $SM = (\mathcal{M}, g, SM, \pi)$  and whose morphisms  $\chi: SM_1 \rightarrow SM_2$  cover a morphism  $\psi: M_1 \rightarrow M_2$  in  $\mathfrak{Spac}$  and satisfy  $\chi \circ (R_1)_S = (R_2)_S \circ \chi$  and  $\pi_2 \circ \chi = \psi_* \circ \pi_1$ , where  $p_i$  are the bundle projections,  $\pi_i$  the spin frame projections and  $\psi_*$  the push-forward.

Note that a morphism acts as a diffeomorphism of the fibers, because it intertwines the group action.

Every globally hyperbolic spacetime admits a spin structure, which need not be unique [6, 8, 19, 21]. We will regard distinct spin structures on the same underlying spacetime as distinct spin spacetimes.<sup>j</sup> Spinor and cospinor fields are sections of vector bundles associated to the spin frame bundle. We will require that the assignment of these vector bundles is functorial:

**Definition 3.3.** A *locally covariant spinor bundle* is a functor  $\mathbf{V}: \mathfrak{S}\mathfrak{Pac} \rightarrow \mathfrak{VBund}_{\mathbb{C}}$ , written as  $SM \mapsto V_{SM}$ ,  $\chi \mapsto \nu$ , such that  $\chi$  and  $\nu$  cover the same morphism  $\psi$  in  $\mathfrak{Spac}$  and such that each  $V_{SM}$  is a vector bundle associated to the spin frame bundle  $SM$  through some representation. The dual functor  $\mathbf{V}^*$  is called a *locally covariant cospinor bundle*. Smooth sections of  $V_{SM}$ , respectively  $V_{SM}^*$ , are called (Dirac) *spinors* (or spinor fields), respectively *cospinors* (cospinor fields).

The condition in the definition of a locally covariant spinor bundle ensures that the vector bundle  $V_{SM}$  and the spin frame bundle  $SM$  are both bundles over the same spacetime  $M$ .

For definiteness we pick out the following standard choice of locally covariant spinor and cospinor bundles:

**Definition 3.4.** The *standard locally covariant Dirac spinor bundle*  $\mathbf{D}_0: \mathfrak{S}\mathfrak{Pac} \rightarrow \mathfrak{VBund}_{\mathbb{C}}$  is the locally covariant spinor bundle which associates to each object  $SM$  of  $\mathfrak{S}\mathfrak{Pac}$  the associated vector bundle  $D_0M = SM \times_{Spin_{1,3}^0} \mathbb{C}^4$  of  $SM$  with the

<sup>j</sup>There exists another approach to spinors, which considers on each spacetime the Clifford bundle. This Clifford bundle is functorial in its dependence on the spacetime, but it does not generally define a spin structure. Indeed, at each point one can identify the Spin group inside the fiber of the Clifford bundle, but there may not be any projection from these Spin groups onto the frame bundle that intertwines the actions of the structure groups, the obstruction being a topological twist. (Conversely, every spin structure can be seen as a topologically twisted copy of the Spin groups in the Clifford bundle.) Nevertheless, it appears to provide sufficient structure to describe all the relevant physics in a functorial way. We refer to [18] for more information on this approach.

representation  $\pi_0$ , and which maps each morphism  $\chi: SM_1 \rightarrow SM_2$  to the morphism  $\xi: D_0M_1 \rightarrow D_0M_2$  given by  $\xi([E, z]) := [\chi(E), z]$ . The *standard locally covariant Dirac cospinor bundle*  $\mathbf{D}_0^*$  is the dual functor of  $\mathbf{D}_0$ .

Recall that a point in  $D_0M$  consists of an equivalence class of pairs  $(E, z) \in SM \times \mathbb{C}^4$ , where the equivalence is given by

$$[R_SE, z] = [E, \pi_0(S)z].$$

The dual functor  $\mathbf{D}_0^*$  then assigns to each  $SM$  the dual vector bundle  $D_0^*M$  whose points are equivalence classes of pairs  $(E, w^*) \in SM \times (\mathbb{C}^4)^*$ , where the equivalence is given by  $[R_SE, w^*] = [E, w^*\pi_0(S^{-1})]$ . (Here we consider  $w^* \in (\mathbb{C}^4)^*$  as a row vector, whereas  $z \in \mathbb{C}^4$  is treated as a column vector.)

For any object  $SM$  the unique connection  $\nabla_{SM}$  on  $TM$  which is compatible with the metric,  $\nabla_{SM}g = 0$ , can be described by an  $l_+^\uparrow$ -valued one-form  $(\Omega_{SM})^b_a$  on the orthonormal frame bundle  $F_+^\uparrow M$  (cf. [22, Chap. 2, Proposition 1.1]), where  $l_+^\uparrow$  is the Lie-algebra of  $\mathcal{L}_+^\uparrow$ , which can be identified with the tangent space of the fiber of  $F_+^\uparrow M$  at any point. For every local section  $e$  of  $F_+^\uparrow M$  the pull-back  $\omega_a^b := e^*(\Omega_{SM}^b_a)$  consists exactly of the connection one-forms of  $\nabla_{SM}$  expressed in the orthonormal frame  $e_a$ . The one-form  $(\Omega_{SM})^b_a$  can be pulled back by the spin frame projection  $\pi$  and lifted to a  $spin_{1,3}^0$ -valued one-form  $\Sigma_{SM}$  on  $SM$ :

$$\Sigma_{SM} := (d\Lambda)^{-1}\pi^*((\Omega_{SM})^b_a) = \frac{1}{4}p^*((\Omega_{SM})^b_a)g_bg^a,$$

where the last equality uses Proposition 2.6. The one-form  $\Sigma_{SM}$  determines a connection on the spin frame bundle  $SM$ . For any associated vector bundle  $DM$  we then find a connection, also denoted by  $\nabla_{SM}$ , determined by the connection one-forms  $\sigma := E^*(\Sigma_{SM})$  in a local section  $E$  of  $SM$ , as represented on  $DM$  (we will give an explicit expression for  $\sigma$  in Eq. (5)). The connection can be viewed as a map  $\nabla_{SM}: C_0^\infty(D_0M) \rightarrow C_0^\infty(T^*M \otimes D_0M)$ , which is a component of a natural transformation<sup>k</sup>  $\nabla: \mathbf{C}_0^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}_0^\infty \circ (\mathbf{T}^* \otimes \mathbf{D}_0)$ . The Leibniz rule allows us to extend it to mixed spinor-tensors, using, e.g.,  $\nabla_a \langle v, u \rangle = \langle \nabla_a v, u \rangle + \langle v, \nabla_a u \rangle$ .

### 3.2. Adjoints, charge conjugation and the Dirac operator

We now define the adjoint and charge conjugation maps on spinors and cospinors. These are special cases of the Fundamental Theorem 2.2, using the complex conjugate and adjoint matrices<sup>l</sup> (cf. [23]).

<sup>k</sup>Alternatively we could have written the connection as a natural transformation from the 1-jet bundle extension of  $\mathbf{D}_0$  to  $\mathbf{T}^* \otimes \mathbf{D}_0$ .

<sup>l</sup>On a general representation space of complex dimension four, one can define many complex conjugations and Hermitean inner products. In order to obtain the desired equalities involving adjoint and charge conjugate spinors later on, we need these two operations to be compatible, i.e.  $\langle \overline{v}, \overline{w} \rangle = \overline{\langle v, w \rangle}$ . Without loss of generality we can then use the standard complex conjugation and Hermitean inner product on  $\mathbb{C}^4$ .

**Theorem 3.5.** *For any irreducible complex representation  $\pi$  of the Dirac algebra  $D$  there are matrices  $A, C \in GL(4, \mathbb{C})$  such that*

$$\begin{aligned} A &= A^*, \quad \pi(g_a)^* = A\pi(g_a)A^{-1}, \quad A n > 0, \\ \bar{C}C &= I, \quad -\overline{\pi(g_a)} = C\pi(g_a)C^{-1} \end{aligned} \quad (3)$$

for all future pointing time-like vectors  $n \in M_0 \subset D$ . We have for all  $S \in Spin_{1,3}^0$ :

$$A = -C^* A^T C,$$

$$\pi(S)^* A \pi(S) = A, \quad \pi(S^{-1}) C^{-1} \overline{\pi(S)} = C^{-1}.$$

Moreover, if  $A', C' \in M(4, \mathbb{C})$  have the properties stated above for the irreducible complex representation  $\pi'$  of  $D$ , then there is an  $L \in GL(4, \mathbb{C})$ , unique up to a sign, such that  $L^* A' L = A$ ,  $(\bar{L})^{-1} C' L = C$  and  $\pi = L^{-1} \pi' L$  on  $D$ .

**Proof.** To prove the existence of  $A$  and  $C$  in the representation  $\pi_0$  we may take  $A = A_0 := \gamma_0$ ,  $C = C_0 := \gamma_2$  and check the required properties straightforwardly. Note for example that

$$\gamma_0 n^a \gamma_a = \begin{pmatrix} n^0 I + n^i \sigma_i & 0 \\ 0 & n^0 I - n^i \sigma_i \end{pmatrix} > 0,$$

because  $\det(n^0 I \pm n^i \sigma_i) = n^2 > 0$  and  $\text{Tr}(n^0 I \pm n^i \sigma_i) = 2n^0 > 0$ . To prove the existence of  $A$  and  $C$  in a general irreducible complex representation  $\pi$  one writes  $\gamma_a = K \pi(g_a) K^{-1}$  by Theorem 2.2 and verifies that  $A = K^* A_0 K$  and  $C = \bar{K}^{-1} C_0 K$  will do.

Given  $A', C'$  satisfying Eq. (3) for  $\pi'$  we can fix  $K \in GL(4, \mathbb{C})$  such that  $\pi' = K \pi K^{-1}$  on  $D$  and the desired matrix  $L$  must be  $L = zK$  for some  $z \neq 0$  by the Fundamental Theorem 2.2. Now set  $\tilde{A} := K^* A' K$  and  $\tilde{C} := (\bar{K})^{-1} C' K$  and note that  $\tilde{A}$  and  $\tilde{C}$  satisfy (3) for  $\pi$ . Because the sets of matrices  $\pi(g_a)^*$  and  $-\overline{\pi(g_a)}$  both satisfy the relations (1) we must have  $aA = \tilde{A}$  and  $cC = \tilde{C}$  for some non-zero complex factors  $a$  and  $c$ , again by the Fundamental Theorem. Also,  $|c| = 1$  because  $\bar{C}C = I$  and  $a > 0$  because  $A = A^*$  and  $A\pi(n) > 0$  for future pointing time-like vectors. Hence,  $|z|^2 = a$  and  $z = c\bar{z}$ , which fixes  $z$  (and  $L$ ) up to a sign. This proves the last statement.

The equation  $A = -C^* A^T C$  holds for  $A_0, C_0$  and therefore also in general. For a unit vector  $u = u^a g_a$  we have  $u^2 = \pm I$  and hence

$$\pi(u)^* A \pi(u) = u^a u^b \pi(g_a)^* A \pi(g_b) = u^a u^b A \pi(g_a g_b) = A \pi(u^2) = \pm A.$$

For  $S \in Spin_{1,3}$ , we must therefore have that  $\pi(S)^* A \pi(S) = \pm A$ , by definition of the Spin group. For  $S = I$ , the sign is a plus, so by continuity and connectedness we conclude that  $\pi(S)^* A \pi(S) = A$  for all  $S \in Spin_{1,3}^0$ . For  $C$ , we use the fact that

$$\pi(u^{-1}) C^{-1} \overline{\pi(u)} = -\pi(u)^{-1} \pi(u) C^{-1} = -C^{-1}$$

and hence  $\pi(S^{-1}) C^{-1} \overline{\pi(S)} = C^{-1}$  for all  $S \in Spin_{1,3}$ . □

Note that  $g_5 \in Spin_{1,3} \setminus Spin_{1,3}^0$ . Indeed, using  $\pi_0$  and  $A_0 = \gamma_0$  in Theorem 3.5 we see that  $\gamma_5^* A_0 \gamma_5 = -A_0$ , so  $g_5 \in Spin_{1,3}$  by definition, but not in  $Spin_{1,3}^0$ .

In the following theorem we use the fact that for any pair of natural transformations  $t, t': \mathfrak{S}\mathfrak{S}\mathfrak{p}\mathfrak{a}\mathfrak{c} \Rightarrow \mathfrak{V}\mathfrak{B}\mathfrak{u}\mathfrak{n}\mathfrak{d}'_{\mathbb{C}}$  we can define the sum  $t + t'$  and the tensor product  $t \otimes t'$  componentwise.

**Theorem 3.6.** *The standard locally covariant Dirac spinor and cospinor bundles admit natural ( $\mathbb{C}$ -antilinear) equivalences  ${}^+\mathbf{D}_0 \Leftrightarrow \mathbf{D}_0^*$ ,  ${}^c\mathbf{D}_0 \Leftrightarrow \mathbf{D}_0$ ,  ${}^c\mathbf{D}_0^* \Leftrightarrow \mathbf{D}_0^*$  in  $\mathfrak{V}\mathfrak{B}\mathfrak{u}\mathfrak{n}\mathfrak{d}_{\mathbb{R}}$  and a natural transformation  $\gamma: \mathbf{D}_0 \Rightarrow \mathbf{T}^* \otimes \mathbf{D}_0$  in  $\mathfrak{V}\mathfrak{B}\mathfrak{u}\mathfrak{n}\mathfrak{d}'_{\mathbb{C}}$  such that all components cover the identity morphism and the following equations hold both on spinors and cospinors (i.e. we denote the inverses of  ${}^+$  and  ${}^c$  by the same symbol):*

$$\begin{aligned} {}^+\circ{}^+ &= 1 = {}^c\circ{}^c, & {}^+\circ{}^c &= -1 \circ{}^c\circ{}^+ \\ \langle, \rangle \circ S \circ ({}^+\otimes{}) &= {}^-\circ\langle, \rangle = \langle, \rangle \circ ({}^c\otimes{}^c) \\ (1\otimes{}) \circ \gamma &= \gamma^*\circ{}^+, & (1\otimes{}^c) \circ \gamma &= -1 \circ \gamma\circ{}^c \\ (1 + S \otimes 1) \circ (1 \otimes \gamma) \circ \gamma &= (2 \circ g) \otimes 1 \\ \nabla \circ \gamma &= \gamma \circ \nabla, \end{aligned} \tag{4}$$

where  $S: \mathbf{D}_0 \otimes \mathbf{D}_0^* \Leftrightarrow \mathbf{D}_0^* \otimes \mathbf{D}_0$  and  $S: \mathbf{T}^* \otimes \mathbf{T}^* \Leftrightarrow \mathbf{T}^* \otimes \mathbf{T}^*$  swap the factors in the tensor product,  $g: \Lambda^0 \Rightarrow \mathbf{T}^* \otimes \mathbf{T}^*$  maps the function 1 to the metric  $g$  and  $\gamma^*: \mathbf{D}_0^* \Rightarrow \mathbf{T}^* \otimes \mathbf{D}_0^*$  is the adjoint map of  $\gamma$  under the canonical pairing  $\langle, \rangle$ . Furthermore, for every object  $SM$ , every time-like future pointing tangent vector  $n \in TM$  and every  $v \in D_0M$  we have  $\langle n \circ v^+, \gamma(v) \rangle \geq 0$ .

The natural transformation  $\gamma$  can also be seen as a natural transformation  $\mathbf{T} \Rightarrow \text{End}(\mathbf{D}_0)$  or  $\mathbf{T} \Rightarrow \text{End}(\mathbf{D}_0^*)$ . Equations (4) simply give the usual computational rules for spinors and cospinors in a functorial setting. Thus, for every  $SM$  and every  $p \in D_0M$ ,  $q \in D_0^*M$  we have:

$$\begin{aligned} p^{++} &= p = p^{cc}, & p^{c+} &= -p^{+c} \\ \langle p^+, q^+ \rangle &= \overline{\langle q, p \rangle} = \langle q^c, p^c \rangle \\ (\gamma_\mu p)^+ &= p^+ \gamma_\mu, & (\gamma_\mu p)^c &= -\gamma_\mu p^c \\ \gamma_\mu \gamma_\nu + \gamma_\nu \gamma_\mu &= 2g_{\mu\nu} I, & \nabla_a \gamma_b &\equiv 0, \end{aligned}$$

where we have dropped the subscript  $SM$  to lighten the notation.

**Proof.** The canonical pairing  $\langle, \rangle: \mathbf{D}_0^* \otimes \mathbf{D}_0 \Rightarrow \Lambda_{\mathbb{C}}^0$  on  $SM$  is given by  $\langle [E, w^*], [E, z] \rangle = \langle w, z \rangle$ , where the right-hand side is the standard Hermitean inner product on  $\mathbb{C}^4$ . Note that this is well-defined, because we can always get the same  $E \in SM$  on the left-hand side by a suitable action of  $Spin_{1,3}^0$ . The components of the natural equivalences  ${}^+$  and  ${}^c$  on each  $SM$  are defined using the matrices  $A_0$  and  $C_0$  of Theorem 3.5 and their properties:

$$\begin{aligned} [E, z]^c &:= [E, C_0^{-1} \bar{z}], & [E, w^*]^c &:= [E, \bar{w}^* C_0], \\ [E, z]^+ &:= [E, z^* A_0], & [E, w^*]^+ &:= [E, A_0^{-1} w]. \end{aligned}$$

These are well-defined isomorphisms in  $\mathfrak{WBund}_{\mathbb{R}}$  and they give rise to natural equivalences satisfying the first two lines of Eq. (4).

Now fix  $E \in SM$ , let  $e_a$  be the orthonormal basis  $(e_0, \dots, e_3) = \pi(E)$  of  $T_{p(E)}M$ , where  $\pi: SM \rightarrow FM$  is the spin frame projection, and let  $e^a$  be the dual basis of  $T_{p(E)}^*M$ . On  $SM$  we define the component of the natural transformation  $\gamma$  on  $SM$  to be

$$\gamma([E, z]) := e^a \otimes [E, \gamma_a z].$$

This is well-defined, because a different section  $E' := R_S E$  gives rise to the frame  $e'_a = e_b \Lambda^b{}_a(S)$  and the dual frame  $(e')^a = \Lambda^a{}_b(S^{-1})e^b$  and on the other hand  $\pi_0(S^{-1})\gamma_a\pi_0(S) = \gamma_b\Lambda^b{}_a(S^{-1})$  by definition of  $\Lambda$  (Proposition 2.6).  $\gamma$  is indeed a morphism in  $\mathfrak{WBund}'_{\mathbb{C}}$  and gives rise to a natural transformation. The third line of Eq. (4) follows again from the properties of  $A$  and  $C$  (see Theorem 3.5):

$$\begin{aligned}\gamma([E, z]^c) &= e^a \otimes [E, \gamma_a C_0^{-1} \bar{z}] = -e^a \otimes [E, C_0^{-1} \overline{\gamma_a z}] = -(\gamma([E, z]))^c, \\ \gamma^*([E, z]^+) &= e^a \otimes [E, z^* A_0 \gamma_a] = e^a \otimes [E, z^* \gamma_a^* A] = (\gamma([E, z]))^+\end{aligned}$$

and similarly on cospinors. Also,

$$\begin{aligned}\nabla_b \gamma_a &= \sigma_b \gamma_a - \gamma_a \sigma_b - \Gamma^c{}_{ba} \gamma_c = \frac{1}{4} \Gamma^c{}_{bd} (\gamma_c \gamma^d \gamma_a - \gamma_a \gamma_c \gamma^d) - \Gamma^c{}_{ba} \gamma_c \\ &= \frac{1}{4} \Gamma^c{}_{bd} (\gamma_c \{\gamma^d, \gamma_a\} - \{\gamma_a, \gamma_c\} \gamma^d - 4\delta_a^d \gamma_c) = \frac{-1}{2} \Gamma^c{}_{bd} (\delta_a^d \gamma_c + \eta_{ac} \gamma^d) = 0.\end{aligned}$$

Finally, for every object  $SM$ , every future pointing tangent vector  $n \in TM$  and every  $v \in D_0 M$  we have  $\langle n \otimes v^+, \gamma(v) \rangle = \langle v^+, A n^a \gamma_a v \rangle \geq 0$  again by Theorem 3.5.  $\square$

In terms of the Christoffel symbols  $\Gamma_{\mu\nu}^\rho$ , the frame  $e_\rho^a$  and representing  $g_a$  on  $D_0 M$  using the  $\text{End}(D_0 M)$ -valued one-forms  $\gamma$ , the connection one-forms of the spin connection can be expressed as<sup>m</sup>

$$\begin{aligned}\sigma_b &:= \frac{1}{4} \Gamma_{bc}^a \gamma_a \gamma^c, \\ \Gamma_{bc}^a &= -e_c^\rho (e_b^\sigma \partial_\sigma e_\rho^a) + e_\rho^a e_b^\mu e_c^\nu \Gamma_{\mu\nu}^\rho.\end{aligned}\tag{5}$$

The Dirac operator is defined on spinors and cospinors by

$$\nabla_{SM} := \gamma^a \nabla_a.$$

This defines natural transformations  $\nabla: \mathbf{C}_0^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}_0^\infty \circ \mathbf{D}_0$ , respectively  $\nabla: \mathbf{C}_0^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{C}_0^\infty \circ \mathbf{D}_0^*$ . The intertwining relations of the adjoint and charge conjugation with the Dirac operator follow from their intertwining with  $\gamma$  in Theorem 3.6:

**Proposition 3.7.**  $\nabla \circ {}^+ = {}^+ \circ \nabla$ ,  $\nabla \circ {}^c = -1 \circ {}^c \circ \nabla$ .

<sup>m</sup>Note the sign error in [6, 7].



**Proof.** Recall that  $^+$  and  $^c$  can be defined pointwise on test-sections. Hence, on any object  $SM$

$$\begin{aligned} (\nabla v)^c &= ((\partial_a v - v \sigma_a) \gamma^a)^c = (\partial_a \bar{v} - \bar{v} \sigma_a) \bar{\gamma}^a C \\ &= -(\partial(\bar{v}C) - \bar{v}C \sigma_a) \gamma^a = -\nabla(\bar{v}C) = -\nabla v^c, \\ (\nabla u)^+ &= (\gamma^a (\partial_a u + \sigma_a u))^+ = (\partial_a u^* + u^* \sigma_a^*) (\gamma^a)^* A \\ &= (\partial_a (u^* A) - u^* A \sigma_a) \gamma^a = \nabla(u^* A) = \nabla u^+, \end{aligned}$$

where the minus sign in the last line appears because the order of the two factors of  $\gamma$  in the expression for  $\sigma_a$  needs to be changed. It follows that  $(\nabla v)^+ = (\nabla v^{++})^+ = (\nabla v^+)^{++} = \nabla v^+$  and  $(\nabla u)^c = (\nabla u^+)^{+c} = -(\nabla u^+)^{c+} = (\nabla u^{+c})^+ = -(\nabla u^c)^+ = -\nabla u^c$ .  $\square$

**Remark 3.8.** A change in the sign convention,  $\tilde{\eta} := -\eta$ , has no physical consequences. In fact, this simply gives rise to  $D \simeq Cl_{3,1}$  as the Dirac algebra, but since  $Cl_{3,1}^0 = Cl_{1,3}^0$  nothing changes in the representation<sup>n</sup> of the group  $Spin_{1,3}^0 = Spin_{3,1}^0$ . To accommodate this change one can set  $\tilde{\gamma}_a := i\gamma_a$  in Eq. (1), which yields the same Dirac algebra and other constructions (although we do get signs for all covectors when raising or lowering indices with  $\tilde{\eta}$ ). This also implies that one should drop the factor  $i$  in front of the Dirac operator in the Dirac equation (6) below, which ensures that  $P_c P = P P_c$  will still be a wave operator. We can also keep the same matrices  $A, C$ , which now must satisfy the relations:

$$-\tilde{\gamma}_a^* = A \tilde{\gamma}_a A^{-1}, \quad \bar{\tilde{\gamma}}_a = C \tilde{\gamma}_a C^{-1}.$$

The spinor and cospinor bundle and the adjoint and charge conjugation maps then remain the same and all the relations between these operations and the Dirac operator remain valid.

### 3.3. The Dirac equation and its fundamental solutions

The Dirac equation on spinor and cospinor fields, respectively, on a spin spacetime  $SM$  is

$$(-i\nabla + m)u = 0, \quad (i\nabla + m)v = 0, \quad (6)$$

where the constant  $m \geq 0$  is to be interpreted as the mass of the field. These equations can be derived as the Euler–Lagrange equations from the action  $\mathcal{S}_D := \int \mathcal{L}_D$

<sup>n</sup>Notice that a complex irreducible representation of  $Cl_{1,3}$  extends to an irreducible representation of  $M(4, \mathbb{C})$  and therefore also gives a complex irreducible representation of  $Cl_{3,1}$  and vice versa. The standard Clifford algebra isomorphism  $Cl_{3,1} \simeq M(4, \mathbb{R})$  appears if and only if the representation of  $Cl_{1,3}$  is a Majorana representation, i.e. if  $\bar{\gamma}_a = -\gamma_a$ . In that case we also find (see, e.g., [12, p. 332])

$$Pin_{3,1} \simeq \{S \in M(4, \mathbb{R}) \mid \det S = 1, \forall v \in M_0 S v S^{-1} \in M_0\} \neq Pin_{1,3}.$$

with the Lagrangian density<sup>o</sup>

$$\mathcal{L}_D := \langle u^+, (-i\nabla + m)u \rangle d\text{vol}_g \quad (7)$$

by varying with respect to  $u$  and  $u^+$ , viewed as independent fields. The canonical momentum of the field  $u$  on a Cauchy surface  $C$  with future pointing normal vector field  $n$  is defined as

$$\pi(x) := \frac{1}{\sqrt{-\det g(x)}} \frac{\delta \mathcal{S}_D}{\delta(n^\mu \nabla_\mu \psi(x))} = -i\psi^+(x)\not{n}(x). \quad (8)$$

We will write  $P := -i\nabla + m$  for the operator on spinors and  $P_c := i\nabla + m$  for the operator on cospinors. These are components of natural transformations  $P: \mathbf{C}_0^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}_0^\infty \circ \mathbf{D}_0$ ,  $P: \mathbf{C}^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0$  and  $P_c: \mathbf{C}_0^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{C}_0^\infty \circ \mathbf{D}_0^*$ ,  $P_c: \mathbf{C}^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0^*$ , which we denote by the same symbol. We then have by Proposition 3.7:

$$\begin{aligned} P \circ {}^c &= {}^c \circ P, & P_c \circ {}^c &= {}^c \circ P_c, \\ P_c \circ {}^{+} &= {}^{+} \circ P, & P \circ {}^{+} &= {}^{+} \circ P_c, \end{aligned} \quad (9)$$

i.e. if a spinor field  $u$  is a solution to the Dirac equation, then so are  $u^+$  and  $u^c$ . (The adjoint and charge conjugation of  $u$  are defined pointwise.)

For a distribution  $v$  on  $D_0M$  we define the transpose  $P^*$  by  $\langle P^*v, u \rangle := \langle v, Pu \rangle$  and similarly for  $P_c$ . In this way the transposes give rise to natural transformations  $P^*: \mathbf{Distr} \circ \mathbf{D}_0 \Rightarrow \mathbf{Distr} \circ \mathbf{D}_0$  and  $P_c^*: \mathbf{Distr} \circ \mathbf{D}_0^* \Rightarrow \mathbf{Distr} \circ \mathbf{D}_0^*$ .

**Lemma 3.9.** *Let  $\iota: \mathbf{C}^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{Distr} \circ \mathbf{D}_0$  and  $\iota: \mathbf{C}^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{Distr} \circ \mathbf{D}_0^*$  be the canonical natural transformations (see the end of Sec. 2.2). Then  $P^* \circ \iota = \iota \circ P_c$  and  $P_c^* \circ \iota = \iota \circ P$ .*

**Proof.** This follows from the fact that for each object  $SM$   $\int_M \langle u, \nabla v \rangle d\text{vol}_g = -\int_M \langle \nabla u, v \rangle d\text{vol}_g$  if at least one of  $u \in C^\infty(D_0M)$  and  $v \in C^\infty(D_0^*M)$  is compactly supported. This in turn follows from  $\langle \nabla v, u \rangle + \langle v, \nabla u \rangle = \nabla_a \langle v, \gamma^a u \rangle$  and Gauss' law.  $\square$

One can find unique advanced and retarded fundamental solutions for the Dirac equation, both for spinors and cospinors [6, 24]:

**Theorem 3.10.** *There are unique natural transformations  $S^\pm: \mathbf{C}_0^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0$  and  $S_c^\pm: \mathbf{C}_0^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0^*$  such that  $S^\pm \circ P = P \circ S^\pm = \kappa$ ,  $S_c^\pm \circ P_c = P_c \circ S_c^\pm = \kappa$  and such that for each  $u \in C_0^\infty(D_0M)$ ,  $v \in C_0^\infty(D_0^*M)$  we have*

<sup>o</sup>The Lagrangian is a natural transformation between the functor  $\mathbf{J}_1\mathbf{D}_0$ , which assigns to each spin spacetime  $SM$  the first-order jet bundle  $J_1D_0M$  of the spinor bundle  $D_0M$ , to the functor  $|\Lambda^n|$  of densities. A component of this natural transformation covers the identity morphism of  $SM$  and is only a morphism in  $\mathbf{Bund}$ , not in  $\mathbf{VBund}_{\mathbb{R}}$ , because it is not linear.

$\text{supp}(S^\pm u) \subset J^\pm(\text{supp}(u))$ ,  $\text{supp}(S_c^\pm u) \subset J^\pm(\text{supp}(u))$ . Moreover,

$$\begin{aligned} S^\pm \circ {}^c &= {}^c \circ S^\pm, & S_c^\pm \circ {}^c &= {}^c \circ S_c^\pm, \\ S_c^\pm \circ {}^+ &= {}^+ \circ S_c^\pm, & S^\pm \circ {}^+ &= {}^+ \circ S^\pm, \\ \int \circ \langle, \rangle \circ (1 \otimes S^\pm) &= \int \circ \langle, \rangle \circ (S_c^\mp \otimes 1). \end{aligned}$$

**Proof.** The components of  $S^\pm$  and  $S_c^\pm$  are the advanced  $(-)$  and retarded  $(+)$  fundamental solutions for  $P$  and  $P_c$ , which are given by  $S^\pm := (i\nabla + m)E^\pm$  and  $S_c^\pm := (-i\nabla + m)E^\pm$  respectively, where  $E^\pm$  are the unique advanced and retarded fundamental solutions for the normally hyperbolic operator  $(i\nabla + m)(-i\nabla + m) = (-i\nabla + m)(i\nabla + m) = \nabla^2 + m^2$ . We refer to [6, Theorem 2.1] for a detailed proof of the existence and uniqueness of these operators (see also [16] for the existence and uniqueness of  $E^\pm$ ).

The naturality of  $S^\pm$  and  $S_c^\pm$  follows from their uniqueness and the naturality of  $P$  and  $P_c$ . In detail: for every morphism  $\chi: SM_1 \rightarrow SM_2$  and every  $f \in C_0^\infty(D_0 M_1)$  the unique smooth solution to  $Pu = \chi_* f$  on  $M_2$  with  $\text{supp}(u) \subset J^\pm(\text{supp}(\chi_* f))$  pulls back to a solution  $v := \chi^* u$  of  $Pv = f$  on  $M_1$  with  $\text{supp}(v) \subset J^\pm(\text{supp}(f))$ . By uniqueness we must then have  $u = S^\pm \chi_* f$  and  $\chi^* u = S^\pm f$ , i.e.  $\chi^* \circ S^\pm \circ \chi_* = S^\pm$ . The same holds for cospinors. The commutation of  $S^\pm$  and  $S_c^\pm$  with charge conjugation and adjoints follows from Eq. (9).

For arbitrary  $u \in C_0^\infty(D_0 M)$  and  $v \in C_0^\infty(D_0^* M)$  we can find a  $\phi \in C_0^\infty(M)$  which is identically one on the compact set  $\text{supp}(S^\pm u) \cap \text{supp}(S_c^\mp v)$ . We then compute:

$$\begin{aligned} \int_M \langle v, S^\pm u \rangle &= \int_M \langle P_c S_c^\mp v, \phi S^\pm u \rangle = \int_M \langle S_c^\mp v, P \phi S^\pm u \rangle \\ &= \int_M \langle S_c^\mp v, \phi P S^\pm u \rangle = \int_M \langle S_c^\mp v, u \rangle, \end{aligned}$$

which proves the last claim.  $\square$

We define the advanced-minus-retarded fundamental solutions  $S := S^- - S^+$  and  $S_c := S_c^- - S_c^+$ , which are natural transformations  $S: \mathbf{C}_0^\infty \circ \mathbf{D}_0 \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0$  and  $S_c: \mathbf{C}_0^\infty \circ \mathbf{D}_0^* \Rightarrow \mathbf{C}^\infty \circ \mathbf{D}_0^*$  respectively.

### 3.4. The non-uniqueness of the functorial Dirac structure

We have seen that the (standard) structure of Dirac spinors and cospinors, adjoints, charge conjugation and the Dirac operator is entirely determined by the functor  $D_0$  and the natural equivalences  ${}^+, {}^c$  and  $\gamma$ . We formalise this with a definition:

**Definition 3.11.** By a *Dirac structure*  $\mathcal{D} := (\mathbf{D}, {}^+, {}^c, \gamma)$  we mean a locally covariant spinor bundle  $\mathbf{D}$  with a dual bundle  $\mathbf{D}^*$ , natural equivalences  ${}^+: \mathbf{D} \Leftrightarrow \mathbf{D}^*$ ,  ${}^c: \mathbf{D} \Leftrightarrow \mathbf{D}$ ,

and  ${}^c\mathbf{D}^* \Leftrightarrow \mathbf{D}^*$  in  $\mathfrak{VBund}_{\mathbb{R}}$  and a natural transformation  $\gamma: \mathbf{D} \Rightarrow \mathbf{T}^* \otimes \mathbf{D}$  in  $\mathfrak{VBund}'_{\mathbb{C}}$ , all of whose components cover the identity morphism and satisfying the relations (4) and  $\langle \gamma_{SM}(v^+, v), n \rangle \geq 0$  for every time-like future pointing vector  $n \in TM$ .

We call  $\mathcal{D}_0 := (\mathbf{D}_0, {}^{+,c}, \gamma)$  of Theorem 3.6 the *standard Dirac structure*.

The category  $\mathfrak{DStruc}$  has all Dirac structures as objects and its morphisms  $t: \mathcal{D}_1 \rightarrow \mathcal{D}_2$  are all natural transformations  $t: \mathbf{D}_1 \Rightarrow \mathbf{D}_2$  whose components are injective morphisms covering the identity morphism and intertwining the adjoints, charge conjugation and  $\gamma$  as follows:

$${}^{+2} \circ t = t \circ {}^{+1}, \quad {}^{c2} \circ t = t \circ {}^{c1}, \quad \gamma_2 \circ (t \otimes t) = \gamma_1.$$

For each Dirac structure, one can perform the constructions of Sec. 3.3. Because the Dirac algebra  $D$  has a unique irreducible complex representation one might expect that the category  $\mathfrak{DStruc}$  admits a corresponding unique initial object, perhaps up to isomorphism. This is an object from which there exists a morphism into any other object. However, as we will explain in this section there is a certain cohomological obstruction of the category  $\mathfrak{GSpac}$  involved. We will first consider the standard Dirac structure, which would be a good candidate for an initial object, and prove the following weaker property:

**Proposition 3.12.** *Any morphism  $t$  from a Dirac structure  $\mathcal{D}$  to the standard Dirac structure  $\mathcal{D}_0$  is an isomorphism.*

**Proof.** Let  $t: \mathcal{D} \rightarrow \mathcal{D}_0$  be a morphism. By the injectivity of the components of  $t: \mathbf{D} \Rightarrow \mathbf{D}_0$  we see that the complex dimension of the fiber of  $DM$  is at most four. On the other hand, the vector bundles  $DM$  are modules for the Dirac algebra represented by  $\gamma$ . Because this algebra is simple, and because Eqs. (4) exclude the trivial representation, we find that  $DM$  must have complex dimension at least four. Therefore,  $t: \mathbf{D} \Rightarrow \mathbf{D}_0$  must be a natural equivalence and it follows that  $t: \mathcal{D} \rightarrow \mathcal{D}_0$  is an isomorphism.  $\square$

**Corollary 3.13.** *If we construct a Dirac structure  $\mathcal{D}_\pi$  analogous to  $\mathcal{D}_0$ , but using a different representation  $\pi$  and matrices  $A, C$ , then  $\mathcal{D}_\pi$  is isomorphic to  $\mathcal{D}_0$ .*

**Proof.** Because we use the same representation on all spacetimes we can construct a natural equivalence  $t: \mathcal{D}_\pi \Leftrightarrow \mathcal{D}_0$  whose components are of the form  $t_{SM}([E, z]) := [E, Lz]$  for some  $L \in GL(4, \mathbb{C})$  which is independent of  $SM$  (cf. Theorem 3.5).  $\square$

**Corollary 3.14.** *If  $\mathcal{D} := (\mathbf{D}_0, {}^{+,c1}, \gamma')$  is any Dirac structure with the standard locally covariant Dirac spinor bundle  $\mathbf{D}_0$ , then  $\mathcal{D}$  is isomorphic to the standard Dirac structure  $\mathcal{D}_0$ .*

**Proof.** At each point  $x$  in each object  $SM$  we can view  $\gamma'_a$  as matrices that represent the Dirac algebra in a representation  $\pi$ . Using the Fundamental Theorem 2.2, we write  $\gamma'_a = L\gamma_a L^{-1}$  for some  $L(x) \in GL(4, \mathbb{C})$ . As  $\gamma'_a$  is well-defined

on  $\mathbf{D}_0$  we must have  $\pi_0(S)\gamma'_a\pi_0(S^{-1}) = \gamma'_b\Lambda^b_a(S)$  for all  $S \in Spin^0_{1,3}$ . This also holds for the matrices  $\gamma$ , so we conclude from the Fundamental Theorem that  $\pi_0(S)L(x) = c(x)L(x)\pi_0(S)$ , where  $c \equiv 1$  by taking  $S = I$ . We can now define a natural equivalence  $t: \mathbf{D}_0 \Leftrightarrow \mathbf{D}_0$  by  $[E, z] \mapsto [E, L(p(E))z]$  such that  $\gamma' \circ t = t \circ \gamma$ . If we also define  ${}^{+2} := t \circ {}^{+1} \circ t^{-1}$  and  ${}^{c2} := t \circ {}^{c1} \circ t^{-1}$ , then  $\mathcal{D} \Leftrightarrow (\mathbf{D}_0, {}^{+2}, {}^{c2}, \gamma) \Leftrightarrow \mathcal{D}_0$ , where the last equivalence follows from the previous corollary.  $\square$

In fact, the proof of Corollary 3.13 shows that for any  $SM$  the quadruple  $(DM, {}^{+}, {}^c, \gamma)$  is unique up to an isomorphism  $t_{SM}$ , if  $DM$  has four-dimensional complex fibers. The isomorphism  $t_{SM}$  itself, however, is only unique up to a sign. In other words, on each spin spacetime we find a discrete  $\mathbb{Z}_2$ -symmetry that preserves all physical relations.<sup>P</sup>

Consider two Dirac structures  $\mathcal{D}$  and  $\mathcal{D}'$  whose locally covariant spinor bundles  $\mathbf{D}$  and  $\mathbf{D}'$  have four-dimensional complex fibers. Comparing the action of these functors on morphisms of  $\mathfrak{S}\mathfrak{Spac}$  one finds a diagram that commutes up to a sign. The existence of an initial object in the category  $\mathfrak{D}\mathfrak{Struc}$  then boils down to the question whether one can choose signs for all spin spacetimes  $SM$  in such a way that all the diagrams commute. The answer is not at all obvious, but can be neatly formulated in terms of the first Stiefel–Whitney class of the category  $\mathfrak{S}\mathfrak{Spac}$ . To explain this we will briefly recall the definition of cohomology groups for categories (cf. [26]).

If  $\mathfrak{C}$  is any category, we can first build a simplicial set from it called the *nerve* of the category (cf. [27]). A 0-simplex is simply an object of  $\mathfrak{C}$ , a 1-simplex is a morphism between two objects, a 2-simplex is a commutative triangle, etc. We will write  $\Sigma_n$  for the set of all  $n$ -simplices. For  $n \geq 1$  every  $n$ -simplex has  $n + 1$  *faces*, which are described by maps  $\partial_j: \Sigma_n \rightarrow \Sigma_{n-1}$ ,  $0 \leq j \leq n$ , which remove the  $j$ th vertex from the diagram.

To find the cohomology of  $\mathfrak{C}$  with values in an Abelian group<sup>q</sup>  $G$ , we define an *n-cochain* with values in  $G$  to be a map  $v: \Sigma_n \rightarrow G$ . We denote the set of *n-cochains* with values in  $G$  by  $C^n(G)$  and we define the *coboundary* map  $d: C^n(G) \rightarrow C^{n+1}(G)$  by

$$dv(s) := \sum_{j=0}^{n+1} (-1)^j v(\partial_j s), \quad s \in \Sigma_{n+1},$$

where we have written the group operation of  $G$  additively. One checks that  $d^2 = 0$  and defines  $v$  to be *closed* iff  $dv = 0$  and *exact* iff  $v = dt$  for some  $(n - 1)$ -cochain  $t$ . The sets of closed and exact  $n$ -cochains are denoted by  $B^n(G)$  and  $Z^n(G)$ , respectively. They inherit an Abelian group structure from  $G$  and because

<sup>P</sup>This may be compared to [25], who use complex spinor structures and then find a local (gauge) symmetry instead of our more restricted global symmetries.

<sup>q</sup> [26] also considers the non-Abelian case, which is much more involved.

$Z^n(G) \subset B^n(G)$  is necessarily normal one can define the  $j$ th cohomology group as the quotient  $H^n(G) := B^n(G)/Z^n(G)$ .

Now let us return to the study of Dirac structures. Suppose that  $\mathcal{D}$  and  $\mathcal{D}'$  both have four-dimensional complex fibers. Without loss of generality, we may assume that both Dirac structures coincide on each spin spacetime, but the action of their locally covariant spinor bundles on a morphism  $\chi$  agrees only up to a sign  $v(\chi) \in \{\pm 1\}$ . We can view  $v : \chi \mapsto v(\chi)$  as a 1-cochain on the category  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  with values in  $\mathbb{Z}_2 = \{0, 1\}$ , where 0 corresponds to  $+1$  and 1 to  $-1$ . Notice that for a composition of morphisms  $\chi = \chi_1 \circ \chi_2$  we find  $v(\chi) = v(\chi_1) + v(\chi_2)$  in  $\mathbb{Z}_2$ , because the Dirac structures are both functorial. In cohomological terms this means precisely that  $dv = 0$ .

If there is a natural equivalence  $t : \mathcal{D} \Leftrightarrow \mathcal{D}'$ , then the components  $t_{SM}$  are automorphisms of the Dirac structure at each  $SM$ , i.e.  $t_{SM} = \pm 1$ , that compensate for all the minus signs in  $v$ . If we view  $t$  as a 0-cochain with values in  $\mathbb{Z}_2$ , this means exactly that  $v = dt$ . So we have proved:

**Theorem 3.15.** *The number of inequivalent Dirac structures whose locally covariant spinor bundles have four-dimensional complex fibers equals the number of first Stiefel–Whitney classes of the category  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$ , i.e. the number of elements in  $H^1(\mathbb{Z}_2)$ .*

**Remark 3.16.** For scalar and vector fields the problem above can be avoided in a natural way. Taking  $\mathcal{L}_+^\uparrow$  in the defining (four-vector) representation, the vector bundle associated to  $F_+^\uparrow M$  is just the tangent bundle  $TM$ . A morphism in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  determines a unique morphism on the tangent bundle, so no topological obstructions occur. Similarly for the scalar field, where one uses the trivial one-dimensional representation of  $\mathcal{L}_+^\uparrow$ , whose associated vector bundle is  $\Lambda^0(M) = M \times \mathbb{R}$ . Again a morphism in  $\mathfrak{M}\mathfrak{a}\mathfrak{n}^n$  automatically determines a unique morphism on these associated vector bundles, now by the requirement that the volume element is preserved.

In general one is dealing with representations of  $Spin_{1,3}^0$  and associates to each morphism in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  an intertwining operator between such representations. For the associated vector bundles of  $SM$ , the physical requirements that we imposed on the bundle morphisms, concerning the adjoint and charge conjugation maps and  $\gamma$ , reduce the intertwiners exactly to a choice of lifting  $\mathcal{L}_+^\uparrow$  to its double cover. In this way it leads to the same first Stiefel–Whitney class that characterizes the number of spin structures on a manifold. For the general case it is expected that one needs a non-Abelian cohomology theory to quantify the obstruction for finding initial objects.

#### 4. The Locally Covariant Quantum Dirac Field

After our discussion of the classical Dirac field in Sec. 3 we now turn to the quantum Dirac field, its construction, its Hadamard states and its relative Cauchy evolution.

### 4.1. Quantization of the free Dirac field

First, we will quantize the free Dirac field in a generally covariant way and establish some of its properties. For this purpose we also present the main ideas of locally covariant quantum field theory as introduced in [2] (see also [5]).

In the following, any quantum physical system will be described by a topological  $*$ -algebra  $\mathcal{A}$  with a unit  $I$ , whose self-adjoint elements are the observables of the system. An injective and continuous  $*$ -homomorphism expresses the notion of a subsystem, whereas a state is described by a normalized and positive continuous linear functional  $\omega$ , i.e.  $\omega(A^*A) \geq 0$  for all  $A \in \mathcal{A}$  and  $\omega(I) = 1$ . The state space of  $\mathcal{A}$  is the set of all states and is denoted by  $\mathcal{A}_1^{*+}$ . Every state gives rise to a GNS-representation  $\pi_\omega$  (see [28, Theorem 8.6.2.]), which is characterized uniquely, up to unitary equivalence, by the GNS-quadruple  $(\pi_\omega, \mathcal{H}_\omega, \Omega_\omega, \mathcal{D}_\omega)$ . Here  $\mathcal{H}_\omega$  is the Hilbert space on which  $\pi_\omega(\mathcal{A})$  acts as (possibly unbounded) operators with the dense, invariant domain  $\mathcal{D}_\omega := \pi_\omega(\mathcal{A})\Omega_\omega$ . The vector  $\Omega_\omega$  is cyclic and satisfies  $\omega(A) = \langle \Omega_\omega, \pi_\omega(A)\Omega_\omega \rangle$  for all  $A \in \mathcal{A}$ .

The collection of all systems forms a category  $\mathfrak{TAlg}$ :

**Definition 4.1.** The category  $\mathfrak{TAlg}$  has as its objects all unital topological  $*$ -algebras  $\mathcal{A}$  and as its morphisms all continuous and injective  $*$ -homomorphisms  $\alpha$  such that  $\alpha(I) = I$ .

A *locally covariant quantum field theory* is a (covariant) functor  $\mathbf{A}: \mathfrak{SSpac} \rightarrow \mathfrak{TAlg}$ , written as  $SM \mapsto \mathcal{A}_{SM}, \chi \mapsto \alpha_\chi$ .

A locally covariant quantum field theory  $\mathbf{A}$  is called *causal* if and only if any pair of morphisms  $\psi_i: SM_i \rightarrow SM, i = 1, 2$ , such that  $\psi_1(\mathcal{M}_1) \subset (\psi_2(\mathcal{M}_2))^\perp$  in  $\mathcal{M}$  yields  $[\alpha_{\psi_1}(\mathcal{A}_{SM_1}), \alpha_{\psi_2}(\mathcal{A}_{SM_2})] = \{0\}$  in  $\mathcal{A}_{SM}$ .

A locally covariant quantum field theory  $\mathbf{A}$  satisfies the *time-slice axiom* iff for all morphisms  $\psi: SM_1 \rightarrow SM_2$  such that  $\psi(\mathcal{M}_1)$  contains a Cauchy surface for  $\mathcal{M}_2$  we have  $\alpha_\psi(\mathcal{A}_{SM_1}) = \mathcal{A}_{SM_2}$ .

Notice that the condition  $\psi_1(\mathcal{M}_1) \subset (\psi_2(\mathcal{M}_2))^\perp$  is symmetric in  $i = 1, 2$ . The causality condition formulates how the quantum physical system interplays with the classical gravitational background field, whereas the time-slice axiom expresses the existence of a causal dynamical law.

We now fix a choice of Dirac structure  $\mathcal{D} := (\mathbf{D}, ^+, ^c, \gamma)$ , in order to turn the free Dirac field into a locally covariant field theory. Because we want to impose the canonical anti-commutation relations it will also be convenient to quantize spinor and cospinor fields simultaneously by introducing the following terminology:

**Definition 4.2.** The *locally covariant double spinor bundle* is the covariant functor  $D \oplus D^*$ . We define the following natural equivalences and natural transformations

on this bundle, indicated by their components at  $SM$ :

$$\begin{aligned}(p \oplus q)^c &:= p^c \oplus q^c, & (p \oplus q)^+ &:= q^+ \oplus p^+, \\ \gamma_\mu(p \oplus q) &:= (\gamma_\mu p) \oplus (\gamma_\mu q), & \langle p \oplus q, p' \oplus q' \rangle &:= \langle p^+, p' \rangle + \langle q^+, q' \rangle, \\ \tau(p \oplus q) &:= p \oplus (-q).\end{aligned}$$

A *double spinor (field)* is an element of  $C^\infty(DM \oplus D^*M)$ . A double *test-spinor (field)* is an element of  $C_0^\infty(DM \oplus D^*M)$ . The adjoint, charge conjugation and other operations are defined pointwise. We also define the operator  $P := P \oplus P_c$ , its advanced  $(-)$  and retarded  $(+)$  fundamental solutions  $S^\pm(u \oplus v) := (S^\pm u) \oplus (S_c^\pm v)$  and  $S := S^- - S^+$ .

The *exterior tensor product*  $\mathcal{V}_1 \boxtimes \mathcal{V}_2$  of two vector bundles  $\mathcal{V}_i$  with fiber  $V_i$  over manifolds  $\mathcal{M}_i$ ,  $i = 1, 2$ , is the vector bundle over  $\mathcal{M}_1 \times \mathcal{M}_2$  whose fiber is  $V_1 \otimes V_2$  and whose local trivializations are determined by  $(O_1 \times O_2) \times (V_1 \otimes V_2)$ , where  $O_i \times V_i$  are local trivializations of  $\mathcal{V}_i$ .

The *Dirac Borchers–Uhlmann algebra*  $\mathcal{F}_{SM}^0$  on a spin spacetime  $SM$  is the topological  $*$ -algebra

$$\mathcal{F}_{SM}^0 := \bigoplus_{n=0}^{\infty} C_0^\infty((DM \oplus D^*M)^{\boxtimes n}),$$

where the direct sum is algebraic (i.e. only finitely many non-zero summands are allowed) and

- (1) the product is given by continuous linear extension of  $f_1 \cdot f_2 := f_1 \boxtimes f_2$ ,
- (2) the  $*$ -operation is given by continuous antilinear extension of

$$(f_1 \boxtimes \cdots \boxtimes f_n)^* := f_n^+ \boxtimes \cdots \boxtimes f_1^+,$$

- (3) as a topological vector space  $\mathcal{F}_{SM}^0$  is the strict inductive limit  $\mathcal{F}_{SM}^0 = \bigcup_{N=0}^{\infty} \bigoplus_{n=0}^N C_0^\infty((DM \oplus D^*M)^{\boxtimes n}|_{K_N^{\times n}})$ , where  $K_N$  is an exhausting and increasing sequence of compact subsets of  $\mathcal{M}$  and the test-section space of the restricted vector bundle  $(DM \oplus D^*M)^{\boxtimes n}|_{K_N^{\times n}}$  is given the test-section topology.

The topology of  $\mathcal{F}_{SM}^0$  is such that a state is given by a sequence of  $n$ -point distributional sections  $\omega_n$  of  $(DM \oplus D^*M)^{\boxtimes n}$ . A morphism  $\chi: SM_1 \rightarrow SM_2$  in  $\mathfrak{SSpac}$  determines a unique morphism  $\alpha_\chi: \mathcal{F}_{SM_1}^0 \rightarrow \mathcal{F}_{SM_2}^0$  that is given by the algebraic and continuous extension of the morphism  $DM_1 \oplus D^*M_1 \rightarrow DM_2 \oplus D^*M_2$  that is supplied by the functor  $\mathbf{D}$ . Together with this map on morphisms the map  $SM \mapsto \mathcal{F}_{SM}^0$  becomes a locally covariant quantum field theory  $\mathbf{F}^0: \mathfrak{SSpac} \rightarrow \mathfrak{Alg}$ . Our next task will be to divide out the ideals that generate the dynamics and the canonical anti-commutation relations.

We define the natural transformation  $(\ , \ ) : (C_0^\infty \circ (\mathbf{D} \oplus \mathbf{D}^*)) \otimes_{\mathbb{R}} (C_0^\infty \circ (\mathbf{D} \oplus \mathbf{D}^*)) \Rightarrow \mathbb{C}$  whose components are the sesquilinear forms:

$$(f_1, f_2) := i \int_M \langle f_1, \tau S f_2 \rangle.$$



Note that this is indeed a natural transformation, because it can be written as a composition of natural transformations including  $\int$ ,  $\langle \cdot, \cdot \rangle$ ,  $+$  and  $\kappa$ .

**Lemma 4.3.** *On each object  $SM$  the sesquilinear form  $(\cdot, \cdot)$  is Hermitean,  $\overline{(f_1, f_2)} = (f_1^c, f_2^c) = (f_2, f_1)$ , and there holds  $(f_1^+, f_2^+) = (f_2, f_1)$ . For any spacelike Cauchy surface  $C \subset M$  with future pointing unit normal vector field  $n^a$  we have*

$$(u_1 \oplus v_1, u_2 \oplus v_2) = \int_C \langle (Su_1)^+, \not{u}(Su_2) \rangle + \langle S_c v_2, \not{u}(S_c v_1)^+ \rangle. \quad (10)$$

**Proof.** The symmetry properties follow straightforwardly from the computational rules of Theorems 3.6 and 3.10. For the last statement we also need a partial integration (see, e.g., [20, Eq. (B.2.26)] for Gauss' law) and we use the Dirac equation:

$$\begin{aligned} & (u_1 \oplus v_1, u_2 \oplus v_2) \\ &= i \int_{J^+(C)} \langle P_c S_c^- u_1^+, Su_2 \rangle + \langle P_c S_c^- v_2, Sv_1^+ \rangle \\ & \quad + i \int_{J^-(C)} \langle P_c S_c^+ u_1^+, Su_2 \rangle + \langle P_c S_c^+ v_2, Sv_1^+ \rangle \\ &= - \int_{J^+(C)} \nabla_a \langle S_c^- u_1^+, \gamma^a Su_2 \rangle + \nabla_a \langle S_c^- v_2, \gamma^a Sv_1^+ \rangle \\ & \quad - \int_{J^-(C)} \nabla_a \langle S_c^+ u_1^+, \gamma^a Su_2 \rangle + \nabla_a \langle S_c^+ v_2, \gamma^a Sv_1^+ \rangle \\ &= \int_C n_a \langle S_c^- u_1^+, \gamma^a Su_2 \rangle + n_a \langle S_c^- v_2, \gamma^a Sv_1^+ \rangle \\ & \quad - \int_C n_a \langle S_c^+ u_1^+, \gamma^a Su_2 \rangle + n_a \langle S_c^+ v_2, \gamma^a Sv_1^+ \rangle \\ &= \int_C \langle (Su_1)^+, \not{u}(Su_2) \rangle + \langle S_c v_2, \not{u}(S_c v_1)^+ \rangle. \quad \square \end{aligned}$$

From Eq. (10) we notice that  $(\cdot, \cdot)$  is positive semi-definite and hence defines a (degenerate) inner product. We proceed by dividing  $\mathcal{F}_{SM}^0$  by the closed ideal  $J_{SM}$  of  $\mathcal{F}_{SM}^0$  generated by all elements of the form  $Pf$  or  $f_1^+ \cdot f_2 + f_2 \cdot f_1^+ - (f_1, f_2)I$ .

**Theorem 4.4.** *The ideal  $J_{SM}$  is a  $*$ -ideal and for any morphism  $\chi: SM_1 \rightarrow SM_2$  we have  $\alpha_\chi(J_{SM_1}) \subset J_{SM_2}$ . We can define the locally covariant quantum field theory  $\mathbf{F}: \underline{\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}} \rightarrow \underline{\mathfrak{I}\mathfrak{A}\mathfrak{l}\mathfrak{g}}$  which assigns to every spin spacetime  $SM$  the  $C^*$ -algebra  $\mathcal{F}_{SM} := \mathcal{F}_{SM}^0 / J_{SM}$ .*

**Proof.** The elements that generate  $J_{SM}$  are invariant under adjoints and under a morphism they are mapped to elements of the same form. This proves the first statement. It follows that the quotients  $\mathcal{F}_{SM}^0 / J_{SM}$  are topological  $*$ -algebras and

that a morphism  $\alpha_\chi: \mathcal{F}_{SM_1}^0 \rightarrow \mathcal{F}_{SM_1}^0$  descends to the quotients as a well-defined morphism. That each algebra  $\mathcal{F}_{SM}^0/J_{SM}$  has a  $C^*$ -norm follows from the fact that they are the inductive limits of finite-dimensional Clifford algebras ([29]). The morphisms on the quotients are necessarily continuous in the norm and therefore extend to morphisms on the  $C^*$ -algebras  $\mathcal{F}_{SM}$ .  $\square$

**Definition 4.5.** A locally covariant quantum field in the locally covariant vector bundle  $\mathbf{V}$  for the locally covariant quantum field theory  $\mathbf{A}$  is a natural transformation  $\Phi: \mathbf{C}_0^\infty \circ \mathbf{V}^* \Rightarrow \mathbf{f} \circ \mathbf{A}$ , where we let  $\mathbf{f}: \mathfrak{Alg} \rightarrow \mathfrak{Vec}$  be the forgetful functor.

We define the locally covariant quantum fields  $B: \mathbf{D} \otimes \mathbf{D}^* \Rightarrow \mathbf{F}$ ,  $\psi: \mathbf{D}^* \Rightarrow \mathbf{F}$  and  $\psi^+: \mathbf{D} \Rightarrow \mathbf{F}$  by  $B_{SM}(f) := 0 \oplus f \oplus 0 \oplus \cdots + J_{SM}$ ,  $\psi_{SM}(v) := B_{SM}(0 \oplus v)$  and  $\psi_{SM}^+(u) := B_{SM}(u \oplus 0)$ .

That the latter really are locally covariant quantum fields is a consequence of

**Proposition 4.6.** The operator-valued maps  $B_{SM}, \psi_{SM}, \psi_{SM}^+$  are  $C^*$ -algebra-valued distributions and:

- (1)  $P \circ \psi = 0$  and  $P_c \circ \psi^+ = 0$ ,
- (2)  $\psi_{SM}^+(u) = \psi_{SM}(u^+)^*$ ,
- (3)  $\{\psi_{SM}^+(u), \psi_{SM}(v)\} = (v^+ \oplus 0, u \oplus 0)I = -i \int_M \langle v, Su \rangle I$  and the other anti-commutators vanish.

**Proof.** The first item is  $PB_{SM}(f) = B_{SM}(P^*f) = B_{SM}(Pf) = 0$ , where  $P^*$  is the formal adjoint of  $P$ . The last two items follow from the definitions of  $\psi_{SM}$  and  $\psi_{SM}^+$  and the properties of  $B_{SM}$  after a straight-forward computation.

It remains to show that  $\psi_{SM}, \psi_{SM}^+$  are  $C^*$ -algebra-valued distributions, because the result for  $B_{SM}$  then follows. The  $C^*$ -subalgebra of  $\mathcal{F}_{SM}$  generated by  $I, \psi_{SM}(v), \psi(v)^*_{SM}$  is a Clifford algebra which is isomorphic to  $M(2, \mathbb{C})$  and an explicit isomorphism is given by  $\psi_{SM}(v) \mapsto \begin{pmatrix} 0 & \sqrt{c} \\ 0 & 0 \end{pmatrix}$ , where  $c = (0 \oplus v, 0 \oplus v) = -i \int_M \langle v, Sv^+ \rangle > 0$ . It follows that  $\|\psi_{SM}(v)\| = \sqrt{c}$  is the operator norm of the corresponding matrix, i.e.<sup>r</sup>

$$\|\psi_{SM}(v)\|^2 = -i \int_M \langle v, Sv^+ \rangle d\text{vol}_g.$$

In the test-spinor topology we then have continuous maps  $v \mapsto v \oplus v^+ \mapsto -i \int_M \langle v, Sv^+ \rangle$ , from which it follows that  $v \mapsto \psi_{SM}(v)$  is norm continuous, i.e. it is a  $C^*$ -algebra-valued distribution. The proof for  $\psi_{SM}^+$  is analogous.  $\square$

Note that the last two conditions of Proposition 4.6 can also be formulated in terms of natural transformations, because the algebraic operations in  $\mathcal{F}_{SM}$  can be expressed as such. The theory  $\mathbf{F}$  is the quantized free Dirac field and  $\psi$  ( $\psi^+$ ) is

<sup>r</sup>The factor 2 in [7, Remark 2, p. 340] seems to be erroneous.

the locally covariant Dirac (co)spinor field. Alternatively we could have used the algebras  $\mathcal{F}_{SM}^0/J_{SM}$  themselves instead of completing them to  $C^*$ -algebras.

To see that the anti-commutator is the canonical one (cf. [24]) we apply [6, Proposition 2.4(c)] which says that  $S|_{C \times C} = -i\delta\eta$  for a Cauchy surface  $C$  with future pointing normal vector field  $n$ . Comparing with Eq. (8) and using  $\eta^2 = I$  we then find

$$\{-i\psi_{SM}^+(\eta(x)), \psi_{SM}(y)\} = - \int_M \langle y, S\eta x \rangle I = i\delta(y, x)I$$

as expected.

So far our construction depends on the choice of a Dirac structure, although naturally equivalent Dirac structures yield naturally equivalent theories and quantum fields. The following theorem restricts attention to the observable algebra, dividing out the freedom of choice completely and yielding a unique theory, but for many purposes it is not convenient to use it directly because it lacks locally covariant Dirac (co)spinor fields.

**Theorem 4.7.** *Let  $\mathbf{B} : \mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c} \rightarrow \mathfrak{T}\mathfrak{A}\mathfrak{lg}$  be the locally covariant quantum field theory that assigns to each spin spacetime  $SM$  the  $C^*$ -subalgebra of  $\mathcal{F}_{SM}$  generated by all even polynomials in elements  $B(f)$ , with the induced action on morphisms. For all Dirac structures with four-dimensional complex fibers the resulting theories  $\mathbf{B}$  are isomorphic.*

**Proof.** The algebras  $\mathcal{B}_{SM}$  generated by the even polynomials are  $C^*$ -algebras. Morphisms respect evenness and so restrict to morphisms on  $\mathcal{B}$ , making  $\mathbf{B}$  a well-defined locally covariant quantum field theory. Now consider two Dirac structures  $\mathcal{D}$  and  $\mathcal{D}_0$  with associated functors  $\mathbf{F}, \mathbf{B}$  and  $\mathbf{F}_0, \mathbf{B}_0$ . If both Dirac structures have four-dimensional complex fibers, then we infer from the comment below Corollary 3.13 that there are  $*$ -isomorphisms  $\alpha_{SM} : \mathcal{F}_{SM} \rightarrow (\mathcal{F}_0)_{SM}$  such that for any morphism  $\chi : SM_1 \rightarrow SM_2$  we have  $\alpha_{SM_2} \circ \alpha_\chi = \epsilon_\chi \cdot (\alpha_0)_\chi \circ \alpha_{SM_1}$ , where  $\epsilon_\chi = \pm 1$  depends only on  $\chi$ . It follows from the evenness that the  $\alpha_{SM}$  descend to  $*$ -isomorphisms  $\alpha_{SM} : \mathcal{B}_{SM} \rightarrow (\mathcal{B}_0)_{SM}$  that intertwine with the morphisms. Hence,  $\mathbf{B}$  and  $\mathbf{B}_0$  are naturally equivalent.  $\square$

**Proposition 4.8.** *The locally covariant quantum field theory  $\mathbf{B} : \mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c} \rightarrow \mathfrak{T}\mathfrak{A}\mathfrak{lg}$  of Theorem 4.7 is causal and satisfies the time-slice axiom.*

**Proof.** Causality follows from the anti-commutation relations,

$$\begin{aligned} & [B_{SM}(f_1)B_{SM}(f_2), B_{SM}(f_3)] \\ &= B_{SM}(f_1)\{B_{SM}(f_2), B_{SM}(f_3)\} - \{B_{SM}(f_1), B_{SM}(f_3)\}B_{SM}(f_2) \\ &= (f_2, f_3)B_{SM}(f_1) - (f_1, f_3)B_{SM}(f_2), \end{aligned}$$

together with the support properties of  $S$ . For the time-slice axiom, we let  $\chi : SM \rightarrow SM'$  be a morphism in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$ , covering a morphism  $\psi : M \rightarrow M'$  in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$ ,

such that  $N := \psi(M) \subset M'$  contains a Cauchy surface  $C \subset M'$ . Then we can choose Cauchy surfaces  $C^\pm \subset N$  such that  $C^\pm \subset I^\pm(C)$  and a smooth partition of unity  $\phi^+, \phi^-$  with  $\text{supp } \phi^\pm \subset J^\pm(C^\mp)$ . Let  $f \in C_0^\infty(DM \oplus D^*M)$  and write

$$f = P(S^+f - \phi^+Sf) + \tilde{f}, \quad (11)$$

where  $\tilde{f} := P(\phi^+Sf) = -P(\phi^-Sf)$  is supported in  $J^+(C^-) \cap J^-(C^+) \subset N$  and  $\phi^+Sf - S^+f$  has compact support. Hence,  $B_{SM_2}(f) = B_{SM_2}(\tilde{f}) = \alpha_\chi(B_{SM_1}(\chi^*(\tilde{f})))$ . Because the algebra  $\mathcal{F}_{M'}$  is generated by such elements this shows that  $\alpha_\chi$  is a  $*$ -isomorphism.  $\square$

**Remark 4.9.** A Majorana spinor is a spinor  $u$  such that  $u = u^c$ . In this case the adjoint is anti-Majorana:  $u^{+c} = -u^{c+} = -u^+$ . We call a double spinor  $f = u \oplus v$  Majorana iff  $u$  and  $v^+$  are Majorana, which means that  $f^c = \tau f$ . Such spinors are sections of a subbundle of the Dirac spinor bundle, which can be described by a Majorana representation. Notice that every spinor is a unique complex linear combination of Majorana spinors.

To quantize Majorana spinors we note that  $\langle h^c, f \rangle = \langle h^+, f^{c+} \rangle$ . This leads us to define the charge conjugation on the quantized fields<sup>s</sup> by  $\psi^c(v) := \psi^+(v^{c+})$  and  $\psi^{+c}(u) := \psi(u^{c+})$ , or equivalently  $B^c(f) := B(f^{c+}) = B(f^c)^*$ . We impose the Majorana condition  $B^c(f) = B(\tau f)$  by dividing out the ideal generated by all elements of the form  $B(f - \tau f^{c+})$ . More precisely, if  $\mathcal{H}$  is the Hilbert space obtained from  $C_0^\infty(DM \oplus D^*M)$  by dividing out the ideal of double spinors  $f$  for which  $(f, f) = 0$ , then there is an orthogonal decomposition  $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ , where the elements in  $\mathcal{H}_\pm$  satisfy  $\tau f^{c+} = \pm f$ . Indeed, every double spinor can be written as  $f = f_+ + if_-$ , where  $f_\pm := \frac{1}{2}(f \pm \tau f^{c+})$  are in  $\mathcal{H}_\pm$  and the orthogonality follows from Lemma 4.3. For the  $C^*$ -algebraic quantization we then have  $\mathcal{F} = \mathcal{F}_+ \otimes \mathcal{F}_-$ , where  $\mathcal{F}_-$  is the  $C^*$ -algebra of quantized Majorana spinors and  $\mathcal{F}_+$  the  $C^*$ -algebra of quantized anti-Majorana spinors (see [30, Sec. 5.2]). The generators  $\psi(v)$  and  $\psi^+(u)$  of  $\mathcal{F}_-$  satisfy the additional relation  $\psi^c = \psi$  and  $\psi^{+c} = -\psi^+$ .

## 4.2. Hadamard states

After Radzikowski's result [31] that a for a scalar field state is of Hadamard form if and only if its wave front set has a certain form, several people set out to extend this result to the Dirac field, or more general quantum fields [32–34]. All three papers have provided an original contribution in their method of proof, but upon careful analysis they all have minor gaps. We feel that it is justified to comment on this here and to provide the necessary results to fill any remaining gaps.

The most general results are the most recent ones, due to Sahlmann and Verch [34], who set out to prove the equivalence of the Hadamard form of a state, defined in terms of the Hadamard parametrix, with a wave front set condition analogous to the scalar field case. One of the techniques used is the scaling limit, but

<sup>s</sup>Our definition differs slightly from that of [13].

the proof of their Proposition 2.8, which relates the wave front set of a distribution to that of its scaling limit, is in our opinion insufficient (see footnote w). In the Appendix, we prove a similar statement as Proposition A.2, thereby filling any gap in [34] and establishing the desired equivalence on a firm ground. For the Dirac field, Hollands has proved that this wave front set condition implies a specific form of the polarization set ([35, Theorem 4.1]).

The scaling limit result can also be used to find the wave front sets of the advanced and retarded fundamental solutions  $E^\pm$  of normally hyperbolic operators on a globally hyperbolic spacetime, a result that we prove as Theorem A.5. Our proof is largely analogous to the work of Radzikowski and the outcome is in direct analogy to the results of Duistermaat and Hörmander [36] for the scalar case. To find the wave front sets of the fundamental solutions  $S^\pm$  for the Dirac equation we use (and correct) an idea of [35].

Finally, we comment on the results by Kratzert [32], which use a spacetime deformation argument to compute the wave front set and polarization set of Hadamard states. This result has a gap, already identified in [34], concerning the case of points  $(x, \xi; y, \xi')$  where either  $\xi = 0$  or  $\xi' = 0$ , which prevents the propagation of the singularity from the original to the deformed spacetime. This gap can be avoided using either a propagation of Hadamard form result as in [34], or using the commutation or anti-commutation relations and the explicit form of  $WF(E)$ , respectively  $WF(S)$ . The latter argument, which appears to be implicit in Radzikowski's paper [31], works as follows: when  $(x, \xi; y, 0) \in WF(\omega_2)$  then also  $(y, 0; x, \xi) \in WF(\omega_2)$  by the (anti-)commutation relations and the fact that  $WF(E)$  (or  $WF(S)$ ) has no points with either entry equal to 0. Using the calculus of Hilbert-space-valued distributions, Theorem A.4, we then find that both  $(x, \xi; x, -\xi) \in WF(\omega_2)$  and  $(x, -\xi; x, \xi) \in WF(\omega_2)$ . Because  $\xi \neq 0$  (by definition the wave front set does not contain the zero covector) these points can both be propagated into a deformed spacetime, where  $WF(\omega)$  is known to satisfy the required microlocal condition. This, however, leads to a contradiction, because  $WF(\omega_2) \cap -WF(\omega_2) = \emptyset$  and hence  $\xi = 0$ . Therefore,  $WF(\omega_2)$  cannot contain points with one of the covectors equal to 0.

After these historical notes we feel free to define the notion of Hadamard states directly in terms of a wave front set condition, rather than using the Hadamard parametrix. If  $\omega$  is a state on  $\mathcal{F}_{SM}$  then we may consider the GNS-representation  $(\mathcal{H}_\omega, \pi_\omega, \Omega_\omega)$  associated to  $\omega$  and the  $\mathcal{H}_\omega$ -valued distribution on  $DM \oplus D^*M$  defined by:

$$v_\omega(f) := \pi_\omega(B_{SM}(f))\Omega_\omega.$$

**Definition 4.10.** A state  $\omega$  on  $\mathcal{F}_{SM}$  is called *Hadamard* if and only if

$$WF(v_\omega) = \mathcal{N}^+ := \{(x, \xi) \in T^*M \mid \xi^2 = 0, \xi^\mu \text{ is future pointing or } 0\}.$$

A state  $\omega$  on  $\mathcal{B}_{SM}$  is called Hadamard if and only if it can be extended to a Hadamard state on  $\mathcal{F}_{SM}$ . The set of all Hadamard states on  $\mathcal{B}_{SM}$  will be denoted by  $\mathcal{S}_{SM}$ .

Note that every state on  $\mathcal{B}_{SM}$  can be extended to  $\mathcal{F}_{SM}$ , by the Hahn–Banach Theorem and Proposition 4.6. The Hadamard condition is independent of the choice of extension, because it depends solely on the two-point distribution as the following proposition shows (cf. [34], we give a short proof using the more advanced microlocal techniques developed in the Appendix).

**Proposition 4.11.** *For a state  $\omega$  on  $\mathcal{F}_{SM}$  the following conditions are equivalent:*

- (1)  $\omega$  is Hadamard,
- (2)  $WF(v_\omega) \subset \mathcal{N}^+$ ,
- (3) the two-point distribution  $\omega_2(f_1, f_2) := \omega(B_{SM}(f_1)B_{SM}(f_2))$  has

$$WF(\omega_2) = \mathcal{C} := \{(x, -\xi; y, \xi') \in T^*M^{\times 2} \setminus \mathcal{Z} \mid (x, \xi) \sim (y, \xi'), (x, \xi) \in \mathcal{N}^+\},$$

where  $(x, \xi) \sim (y, \xi')$  if and only if there is an affinely parameterized light-like geodesic from  $x$  to  $y$  to which  $\xi, \xi'$  are cotangent,

- (4) there is a two-point distribution  $w$  such that  $\omega_2(f_1, f_2) = iw(Pf_1, f_2)$  and  $WF(w) = \mathcal{C}$ .

**Proof.** First, note that  $\omega_2$  is a bidistribution on  $DM \oplus D^*M$ , because  $B_{SM}$  is an  $\mathcal{F}_{SM}$ -valued distribution and multiplication in  $\mathcal{F}_{SM}$  and  $\omega$  are continuous. By Theorem A.4 the third statement implies the first, which trivially implies the second. To show that the second statement implies the third, we use the argument of [37, Proposition 6.1]. By Theorem A.4 we see that  $WF(\omega_2) \subset \mathcal{N}^- \times \mathcal{N}^+$ , where  $\mathcal{N}^- := -\mathcal{N}^+$ . Defining  $\tilde{\omega}_2(f_1, f_2) := \omega_2(f_2, f_1)$  we find  $WF(\tilde{\omega}_2) \cap WF(\omega_2) = \emptyset$ . Now,  $(\omega_2 + \tilde{\omega}_2)(f_1, f_2) = i \int_M \langle f_1, \tau S f_2 \rangle$ , so  $WF(\omega_2) \cup WF(\tilde{\omega}_2) = WF(S) = WF(E)$  by Proposition A.7 and hence  $WF(\omega_2) = WF(E) \cap \mathcal{N}^- \times \mathcal{N}^+ = \mathcal{C}$  by Corollary A.6.

Now, assume that  $\omega_2(f_1, f_2) = iw(Pf_1, f_2)$ , where  $WF(w) = \mathcal{C}$ . Then  $WF(\omega_2) = WF((P^* \otimes I)w) \subset WF(w) = \mathcal{C}$ . It follows that  $WF(v_\omega) \subset \mathcal{N}^+$ . For the converse we suppose that  $\omega$  is Hadamard and we choose a smooth real-valued function  $\phi^+$  on  $M$  such that  $\phi^+ \equiv 0$  to the past of some Cauchy surface  $C_-$  and such that  $\phi^- := 1 - \phi^+ \equiv 0$  to the future of another Cauchy surface  $C_+$ . We then define  $w(f_1, f_2) := -i\omega_2(\phi^+ S^- f_1 + \phi^- S^+ f_1, f_2)$ . Note that  $w$  is a bidistribution which is well-defined, because  $\phi^+ S^- f_1$  and  $\phi^- S^+ f_1$  are compactly supported. By construction  $iw(Pf_1, f_2) = \omega_2(f_1, f_2)$ . We now estimate the wave front set of  $w$  as follows. The wave front sets of  $S^\pm$  are determined in Proposition A.7. Then we may apply [38, Theorems 8.2.9 and 8.2.13] (in combination with Eq. (17)) to estimate the wave front sets of the tensor products  $\phi^\pm(x)S^\mp(x, y)\delta(x', y')$  and the compositions in  $iw(x, x') = \sum_\pm \int \omega_2(y, y')(\phi^\pm(x)S^\mp(x, y)\delta(x', y'))$  respectively and, using  $WF(\omega_2) = \mathcal{C}$ , we find:

$$WF(iw) \subset \cup_\pm WF(S^\mp \otimes \delta) \circ WF(\omega_2) \subset WF(\omega_2) = WF((P^* \otimes I)w) \subset WF(w),$$

i.e.  $WF(w) = WF(\omega_2) = \mathcal{C}$ . □

The second characterization in Proposition 4.11 is especially useful, because it shows we do not need to compute the entire wave front set, as long as we can estimate it. Employing similar techniques as above one can use the anti-commutation relations and the wave front set of  $\omega_2$  to estimate the wave front sets of all higher  $n$ -point distributions [39], showing that a Hadamard state necessarily satisfies the microlocal spectrum condition ( $\mu$ SC) of [40] and it follows that the set of such states is closed under operations from the algebra. We formulate this and other properties of Hadamard states in the following

**Proposition 4.12.** *The set  $\mathcal{S}_{SM}$  of all Hadamard states on  $\mathcal{B}_{SM}$  satisfies:*

- (1)  $\alpha_\chi^*(\mathcal{S}_{SM_1}) \subset \mathcal{S}_{SM_2}$  for every morphism  $\chi: SM_1 \rightarrow SM_2$ ,
- (2)  $\mathcal{S}_{SM}$  is closed under operations from  $\mathcal{B}_{SM}$ ,
- (3)  $\alpha_\chi^*(\mathcal{S}_{SM_1}) = \mathcal{S}_{SM_2}$  for every morphism  $\chi: SM_1 \rightarrow SM_2$  such that  $\psi(\mathcal{M}_1)$  contains a Cauchy surface of  $\mathcal{M}_2$ .

**Proof.** The first property follows from Theorem 4.11 and the fact that wave front sets are local and geometric objects (cf. [38, Chap. 8]). The second property relies on the anti-commutation relations, which implies that the truncated  $n$ -point distributions are totally anti-symmetric (cf. [1, 39]). The final property follows from the second characterisation in Theorem 4.11, Eq. (17) in the Appendix, the equation of motion and the Propagation of Singularities Theorem for the wave front set, which in this case follows from the propagation of the polarization set [41].  $\square$

One can also prove that the state spaces are locally physically equivalent [5] and that all quasi-free Hadamard states are locally quasi-equivalent [42]. Whether the latter remains true for all Hadamard states appears to be unknown.

We conclude this section with the remark that the functor  $\mathbf{S}: \mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c} \rightarrow \mathfrak{T}\mathfrak{M}\mathfrak{e}\mathfrak{c}$  defined by  $SM \mapsto \mathcal{S}_{SM}$  and  $\chi \mapsto \alpha_\chi^*$  (restricted to the relevant state space) is a locally covariant state space for the theory  $\mathbf{B}$  [2].

### 4.3. The relative Cauchy evolution of the Dirac field and the stress-energy-momentum-tensor

Now that we have a locally covariant free Dirac field at our disposal, we will investigate the idea of relative Cauchy evolution for this field and prove that it yields commutators with the stress-energy-momentum tensor. This result is completely analogous to the result for the free scalar field of [2].

Suppose that we have two objects  $M_0 = (\mathcal{M}, g_0, SM_0, p_0)$  and  $M_g = (\mathcal{M}, g, SM_g, p_g)$  in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$ , where  $\mathcal{M}$  is the same in both cases and such that outside a compact set  $K \subset \mathcal{M}$  we have  $g = g_0$ ,  $SM_g = SM_0$  and  $p_g = p_0$ . Now let  $N^\pm \subset M_0$  be causally convex open regions, each containing a Cauchy surface for  $M_0$ , such that  $K$  lies to the future of  $N^-$  (i.e.  $K \subset J^+(N^-) \setminus N^-$  in  $M_0$  and hence also in  $M_g$ ) and to the past of  $N^+$ . We view  $N^\pm$  as objects in  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  and

consider the canonical morphisms  $\iota_0^\pm: N^\pm \rightarrow M_0$  and  $\iota_g^\pm: N^\pm \rightarrow M_g$ . By the time-slice axiom, Proposition 4.8, these give rise to  $*$ -isomorphisms  $\beta_0^\pm: \mathcal{B}_{N^\pm} \rightarrow \mathcal{B}_{M_0}$  and  $\beta_g^\pm: \mathcal{B}_{N^\pm} \rightarrow \mathcal{B}_{M_g}$ . We then define

$$\beta_g := \beta_0^+ \circ (\beta_g^+)^{-1} \circ \beta_g^- \circ (\beta_0^-)^{-1}.$$

The  $*$ -isomorphism  $\beta_g: \mathcal{B}_{M_0} \rightarrow \mathcal{B}_{M_g}$  measures the change in an operator  $A \in \mathcal{B}_{N^-}$  as it evolves to  $N^+$  in the metric  $g$  instead of  $g_0$ .<sup>t</sup>  $\beta_g$  can be extended to a  $*$ -isomorphism of the algebra  $\mathcal{F}_{M_0}$ , where we fix the signs for the isomorphisms between the spinor bundles involved by identifying the double spinor bundles over  $N^\pm \subset M_0$  and  $N^\pm \subset M_g$ . It represents the *relative Cauchy evolution* of the free Dirac field.

We will want to compute the variation of the  $*$ -isomorphism  $\beta_g$  as well as that of the action for the free Dirac field with respect to the metric  $g$ . For this purpose, we will suppose that the compact set  $K \subset \mathcal{M}$  has a contractible neighborhood  $O$  which does not intersect either  $N^\pm$ . Let  $\epsilon \mapsto g_\epsilon$  be a smooth curve from  $[0, 1]$  into the space of Lorentzian metrics on  $\mathcal{M}$  starting at  $g_0$  and such that  $g_\epsilon = g_0$  outside  $K$  for every  $\epsilon$ . The spin bundle  $SM_\epsilon$  must be trivial over the contractible region  $O$ . If we assume it to be diffeomorphic to  $SM_0$  outside  $K$  we can simply take  $SM_\epsilon = SM_0$  as a manifold and, choosing a fixed representation and matrices  $A, C$ , we obtain  $DM_\epsilon = DM$ .

The deformation of the spin structure is contained entirely in the spin frame projection  $\pi_\epsilon: SM_0 \rightarrow FM_\epsilon$ . Let  $E$  be a section of  $SM_0$  over  $O$  and set  $(e_\epsilon)_a := \pi_\epsilon(E)$ . We require that  $e_\epsilon$  varies smoothly with  $\epsilon$  and that  $(e_\epsilon)_a = (e_0)_a$  outside  $K$ . To show that projections  $\pi_\epsilon$  with these properties exist we can apply the Gram–Schmidt orthonormalisation procedure to  $(e_0)_a$  for all  $\epsilon$  simultaneously. The assignment  $E \mapsto e_\epsilon$  determines  $\pi_\epsilon$  completely, using the intertwining properties. The family of frames  $e_\epsilon$  determines principal fiber bundle isomorphisms  $FM_\epsilon \rightarrow FM_0$  between the frame bundles by

$$\lambda_\epsilon: \{(e_\epsilon)_a\} \mapsto \{(e_0)_a\}$$

on  $K$  and extending it by the identity on the rest of  $\mathcal{M}$ . By definition  $f_\epsilon$  intertwines the action of  $\mathcal{L}_+^\uparrow$  on the orthonormal frame bundles.

**Remark 4.13.** There may be many deformations of the spin structure, i.e. many families of projections  $\pi_\epsilon$  which satisfy our requirements. However, the variation of terms like  $\langle v, P_\epsilon u \rangle$  will not depend on this choice. Indeed, if  $\pi'_\epsilon$  is a different deformation of the spin structure, then  $e'_\epsilon := \pi'_\epsilon(E) = R_{\Lambda_\epsilon} e_\epsilon = \pi_\epsilon(R_{S_\epsilon} E)$  for some smooth curve  $S_\epsilon$  in  $Spin_{1,3}^0$ . However, using the invariance of  $\langle, \rangle$  under the action of the gauge group  $Spin_{1,3}^0$ , the variation will be equal in both cases. (Also  $\delta u = 0$  for

<sup>t</sup>In [2], it seems the authors have the scattering of a state in mind as it passes through the perturbed metric, which leads them to consider the  $*$ -isomorphisms  $\beta_{g^{-1}}$  rather than  $\beta_g$ . When we take the variation with respect to  $g$  this gives rise to a sign.



every spinor  $u$ , because  $D_\epsilon M = DM$ .) In this sense, the variation will only depend on the variation of the metric.

#### 4.3.1. The stress-energy-momentum tensor

The classical stress-energy-momentum tensor for the Dirac field is defined as a variation of the action  $\mathcal{S} = \int_{\mathcal{M}} \mathcal{L}_D$ , with the Lagrangian density (7), with respect to  $g^{\mu\nu}(x)$ :

$$T_{\mu\nu}(x) := \frac{2}{\sqrt{-\det g(x)}} \frac{\delta \mathcal{S}}{\delta g^{\mu\nu}(x)}, \quad (12)$$

where  $\psi$  is a free classical Dirac spinor,  $\psi^+$  its adjoint. An explicit computation yields<sup>u</sup>

$$T_{\mu\nu} = \frac{i}{2} (\langle \psi^+, \gamma_{(\mu} \nabla_{\nu)} \psi \rangle - \langle \nabla_{(\mu} \psi^+, \gamma_{\nu)} \psi \rangle).$$

Here the brackets around indices denote symmetrization as an idempotent operation and in the following indices between  $|\cdots|$  are to be excluded from the symmetrization.

Following [7] we quantize the stress-energy-momentum tensor via a point-split procedure, i.e. we want to find a bi-distribution of scalar test-functions which reduces to  $T_{\mu\nu}$  on the diagonal and which can be quantized in a straight-forward way. For this purpose we use a local spin frame  $E_A$  and recall that the components  $\gamma_a^A$  of  $\gamma_a$  are constant. We define:

$$\begin{aligned} T_{ab}^s(x, y) := & \frac{i}{2} (\langle \psi^+, E_A \rangle(x) \gamma_{(a|B|}^A \langle E^B, e_b^\mu \nabla_\mu \psi \rangle(y) \\ & - \langle e_a^\mu \nabla_{|\mu} \psi^+, E_{A|} \rangle(x) \gamma_{b)B}^A \langle E^B, \psi \rangle(y)), \end{aligned}$$

reduces to  $T_{ab} := e_a^\mu e_b^\nu T_{\mu\nu}$  in the limit  $y \rightarrow x$ . Performing a partial integration,  $\int \nabla_\mu (e_a^\mu \langle v, u \rangle) = 0$ , we can write  $T_{ab}^s$  as a bidistribution of scalar test-functions  $h_1, h_2$ ,

$$\begin{aligned} T_{ab}^s(h_1, h_2) = & \frac{i}{2} (-\psi^+(E_A h_1) \gamma_{(a|B|}^A \psi(\nabla_{\mu|} (E^B e_b^\mu h_2)) \\ & + \psi^+(\nabla_\mu (e_a^\mu E_{|A|} h_1)) \gamma_{b)B}^A \psi(E^B h_2)). \end{aligned} \quad (13)$$

Equation (13) can be promoted to the quantized case by replacing  $\psi$  and  $\psi^+$  by the components  $\psi_{SM}$  and  $\psi_{SM}^+$  of the corresponding locally covariant quantum field. The expression (13) can be viewed as a formal expression for the same distribution with quantized field operators.

<sup>u</sup>For explicit computations, we refer to [43, Sec. 4], which uses a Lagrangian that differs from ours by a total derivative. Varying with respect to  $g_{\mu\nu}$  would yield the opposite sign.

**Proposition 4.14.** *For all  $f \in C_0^\infty(DM \oplus D^*M)$  and  $h \in C_0^\infty(M)$  we have:*

$$\begin{aligned} \int_M [T_{ab}^s(x, x), B_{SM}(f)] h(x) d\text{vol}_g(x) \\ = \frac{1}{2} \{ (\nabla_{(a} B_{SM})(\gamma_b)(S\tau f)h) - B_{SM}(\gamma_{(b} \nabla_{a)}(S\tau f)h) \}, \end{aligned}$$

where  $\nabla_a := e_a^\mu \nabla_\mu$ .

**Proof.** For  $f = u \oplus v$  we use Proposition 4.6 to obtain:

$$\begin{aligned} \{B_{SM}(f), \psi_{SM}^+(E_A h)\} &= -i \int_M \langle v, S E_A h \rangle I = i \int_M \langle S_c v, E_A \rangle h I, \\ \{B_{SM}(f), \psi_{SM}(\nabla_\mu E^B e_b^\mu h)\} &= -i \int_M \langle \nabla_\mu E^B e_b^\mu h, S u \rangle I = i \int_M \langle E^B, e_b^\mu \nabla_\mu S u \rangle h I, \\ \{B_{SM}(f), \psi_{SM}^+(\nabla_\mu e_a^\mu E_A h)\} &= -i \int_M \langle v, S \nabla_\mu e_a^\mu E_A h \rangle I = -i \int_M \langle e_a^\mu \nabla_\mu S_c v, E_A \rangle h I, \\ \{B_{SM}(f), \psi(E^B h)\} &= -i \langle E^B, S u \rangle h I. \end{aligned}$$

With Eq. (13), the commutation relations and  $[AB, C] = A\{B, C\} - \{A, C\}B$  this implies

$$\begin{aligned} [T_{ab}^s(x, y), B_{SM}(f)] &= \frac{1}{2} \{ \psi_{SM}^+(E_A(x)) \gamma_{(a|B|}^A \langle E^B, \nabla_b \rangle S u \rangle(y) \\ &\quad + \langle S_c v, E_A \rangle(x) \gamma_{(a|B|}^A (\nabla_b) \psi_{SM})(E^B(y)) \\ &\quad - (\nabla_{(a} \psi_{SM}^+)(E_{|A|}(x)) \gamma_{b)}^A \langle E^B, S u \rangle(y) \\ &\quad - \langle \nabla_{(a} S_c v, E_{|A|} \rangle(x) \gamma_{b)}^A \psi_{SM}(E^B(y)) \}. \end{aligned}$$

In this expression, we are multiplying distributions with smooth functions, so we may take the coincidence limit yielding:

$$\begin{aligned} [T_{ab}^s(x, x), B_{SM}(f)] &= \frac{1}{2} \{ \psi_{SM}^+(\gamma_{(a} \nabla_{b)}(S u)(x)) + \nabla_{(b} \psi_{SM}(S_c v \gamma_{a)}(x)) \\ &\quad - \nabla_{(a} \psi_{SM}^+(\gamma_{b)} S u(x)) - \psi_{SM}(\nabla_{(a} (S_c v) \gamma_{b)}(x)) \} \\ &= \frac{-1}{2} \{ \nabla_{(a} B_{SM}(\gamma_{b)} S \tau f(x)) - B_{SM}(\gamma_{(b} \nabla_{a)}(S \tau f)(x)) \}, \end{aligned}$$

from which the result follows. □

This result can be written for spinors and cospinors separately as:

$$\begin{aligned}
 & \int_M [T_{ab}^s(x, x), \psi_{SM}(v)] h(x) d\text{vol}_g(x) \\
 &= \frac{1}{2} \{ \nabla_{(a} \psi_{SM}((S_c v) \gamma_b) h) - \psi_{SM}(\nabla_{(a} (S_c v) \gamma_b) h) \}, \\
 & \int_M [T_{ab}^s(x, x), \psi_{SM}^+(u)] h(x) d\text{vol}_g(x) \\
 &= \frac{-1}{2} \{ \nabla_{(a} \psi_{SM}^+(\gamma_b) S u h) - \psi_{SM}^+(\gamma_{(a} \nabla_{b)} (S u) h) \}.
 \end{aligned}$$

#### 4.3.2. Relative Cauchy evolution

To compute the relative Cauchy evolution explicitly, we first note that the isomorphism  $\beta_g$  can be characterized in terms of its action on the generators  $B_{M_0}(f)$  of  $\mathcal{F}_{M_0}$  as follows:

**Proposition 4.15.** *For  $f \in C_0^\infty(DN^+ \oplus D^*N^+)$ , we have  $\beta_g B_0(f) = B_0(T_g f)$ , where*

$$T_g f = P_g \phi_+ S_g P_0 \phi_- S_0 f.$$

Here the subscripts on  $B, P$  and  $S$  indicate whether they are the objects defined on  $M_0$  or  $M_g$  and the smooth functions  $\phi_\pm$  are such that  $\phi_\pm \equiv 1$  to the past of some Cauchy surface in  $N^\pm$  and  $\phi_\pm \equiv 0$  to the future of some other Cauchy surface in  $N^\pm$ .

**Proof.** Note that  $\beta_g^- \circ (\beta_0^-)^{-1} B_0(\tilde{f}) = B_g(\tilde{f})$  for any  $\tilde{f} \in C_0^\infty(DN^- \oplus D^*N^-)$ . Similarly, for  $f' \in C_0^\infty(DN^+ \oplus D^*N^+)$  we have  $\beta_0^+ \circ (\beta_g^+)^{-1} B_g(f') = B_0(f')$ . The functions  $\phi_\pm, 1 - \phi_\pm$  have been chosen appropriately in order to apply Eq. (11) in Proposition 4.8. We then have  $B_0(\tilde{f}) = B_0(f)$ , where  $\tilde{f} := -P_0 \phi_- S_0 f$ . Notice that  $\tilde{f}$  indeed has a compact support in  $N^-$ . Similarly,  $B_g(\tilde{f}) = B_g(f')$ , where  $f' := -P_g \phi_+ S_g \tilde{f}$  has support in  $N^+$ . Hence, for  $f' = T_g f$ :  $\beta_g B_0(f) = \beta_g B_0(\tilde{f}) = \beta_0^+ \circ (\beta_g^+)^{-1} B_g(\tilde{f}) = \beta_0^+ \circ (\beta_g^+)^{-1} B_g(f') = B_0(f')$ .  $\square$

On each spin spacetime  $M_\epsilon = (\mathcal{M}, g_\epsilon, SM_0, \pi_\epsilon)$  we can now quantize the Dirac field and obtain relative Cauchy evolutions  $\beta_\epsilon := \beta_{g_\epsilon}$  on  $\mathcal{F}_{N^+}$  as before.

**Proposition 4.16.** *Writing  $\delta := \partial_\epsilon|_{\epsilon=0}$  we have for all  $f \in C_0^\infty(DN^+ \oplus D^*N^+)$ :*

$$\delta(\beta_\epsilon B_0(f)) = B_0(\tau(\delta \nabla_\epsilon) S_0 f).$$

**Proof.** Using the fact that  $B_0$  is a  $C^*$ -algebra-valued distribution and Proposition 4.15 we find:

$$\begin{aligned}
 \delta(\beta_\epsilon B_0(f)) &= \delta(B_0(P_\epsilon \phi_+ S_\epsilon P_0 \phi_- S_0 f)) \\
 &= B_0(\delta(P_\epsilon \phi_+ S_\epsilon) P_0 \phi_- S_0 f) \\
 &= B_0(\delta(P_\epsilon) \phi_+ S_0 P_0 \phi_- S_0 f) + B_0(P_0 \phi_+ \delta(S_\epsilon) P_0 \phi_- S_0 f).
 \end{aligned}$$

Now, because  $P_0\phi_-S_0f \in C_0^\infty(DN^- \oplus D^*N^-)$  we see that  $\delta(S_\epsilon)P_0\phi_-S_0f$  vanishes on  $J^-(N^-)$  and that  $\phi_+\delta(S_\epsilon)P_0\phi_-S_0f$  has compact support. Because  $B_0$  solves the Dirac equation we conclude that the second term vanishes. The first term can be rewritten using Eq. (11), which yields  $S_0f = -S_0P_0(\phi_-S_0f)$  and hence:

$$\delta(\beta_\epsilon B_0(f)) = -B_0(\delta(P_\epsilon)\phi_+S_0f) = -B_0(\delta(P_\epsilon)S_0f).$$

For the last equality, we used the fact that  $\delta(P_\epsilon)$  is supported in  $K$ , where  $\phi_+ \equiv 1$ . Recall that  $P = (-i\nabla + m) \oplus (i\nabla + m)$  to get the final result.  $\square$

To compute the variation of the Dirac operator we may work in a local frame on  $O$ , where it is supported. Because the Dirac adjoint map is independent of  $\epsilon$  we only need to compute this variation either for spinors or for cospinors:

**Lemma 4.17.** *For  $v \in C_0^\infty(D^*M)$  we have  $\delta(\nabla)v = (\delta(\nabla)v^+)^+$ .*

**Proof.** Because the adjoint operation is continuous we have:

$$\delta(\nabla)v = \partial_\epsilon \nabla_\epsilon v|_{\epsilon=0} = \partial_\epsilon (\nabla_\epsilon v^+)^+|_{\epsilon=0} = (\partial_\epsilon \nabla_\epsilon v^+|_{\epsilon=0})^+ = (\delta(\nabla)v^+)^+. \quad \square$$

It is interesting to note that only the variation of the Dirac operator is of importance for the variation of the relative Cauchy evolution, just like for the stress-energy-momentum tensor (cf. [43]). It will also turn out that the variation only depends on the variation of the metric and not on the other freedom in the variation of the orthonormal frame, even though we are now acting on it with the  $C^*$ -algebra-valued field (cf. Remark 4.13). This will follow from the proof of the following theorem, for which we refer to [Appendix B](#).

**Theorem 4.18.** *For a double test-spinor  $f \in C_0^\infty(DM_0 \oplus D^*M_0)$  and  $x \in K$ :*

$$\frac{\delta}{\delta g^{\alpha\beta}(x)}(\beta_g B_0(f)) = -B_0 \left( \frac{\delta}{\delta g^{\alpha\beta}(x)} P_g S_0 f \right) = \frac{-i}{2} e_\alpha^a e_\beta^b [T_{ab}^s(x, x), B_0(f)]. \quad (14)$$

This result compares well with the scalar field case, [2, Theorem 4.3].<sup>v</sup> As particular cases we obtain for  $\psi$  and  $\psi^+$ :

$$\begin{aligned} \frac{\delta}{\delta g^{\alpha\beta}(x)}(\beta_g \psi(v)) &= \frac{-i}{2} e_\alpha^a e_\beta^b [T_{ab}^s(x, x), \psi(v)], \\ \frac{\delta}{\delta g^{\alpha\beta}(x)}(\beta_g \psi^+(u)) &= \frac{-i}{2} e_\alpha^a e_\beta^b [T_{ab}^s(x, x), \psi^+(u)]. \end{aligned}$$

<sup>v</sup>The sign explained in footnote t cancels the sign due to the variation with respect to  $g^{\alpha\beta}$  instead of  $g_{\alpha\beta}$ .

It follows that the same result also holds for products and sums of smeared field operators.

## 5. Conclusions

A rigorous formulation of quantum field theories in curved spacetime, going beyond the well-known scalar field, is a prerequisite for constructing more realistic cosmological models as well as for improving our understanding of quantum field theory in Minkowski spacetime. The main purpose of this paper was to present the free Dirac field in a four-dimensional globally hyperbolic spacetime as a locally covariant quantum field theory in the sense of [2] and to compute the relative Cauchy evolution of this field, obtaining commutators with the stress-energy-momentum tensor in analogy with the free real scalar field. We achieved this in a representation independent way and in a functorial, and therefore manifestly covariant, framework.

We established some basic properties of the locally covariant free Dirac field and remarked on the quantization of Majorana spinors. We also provided a detailed discussion of Hadamard states, closing any gaps in the existing proofs of the equivalence of the definitions in terms of the series expansion of their two-point distribution and a microlocal condition, respectively.

Furthermore, we argued that the observable part of the theory is uniquely determined by the relations between adjoints, charge conjugation and the Dirac operator, although the geometric constructions themselves may not be unique due to the cohomological properties of the category of spin spacetime. On a mathematical level we have consistently replaced a single spin spacetime  $SM$  by the category  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  of such spacetimes, and the differential geometry on  $SM$  by the corresponding functorial descriptions. On a physical level, however, we should not conclude from this that  $\mathfrak{S}\mathfrak{P}\mathfrak{a}\mathfrak{c}$  is now the physical arena in which our system lives, instead of a collection of systems. (See [1, Chap. 1] for more detailed philosophical remarks on the interpretation of the locally covariant approach.)

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## Appendix A. Results in Microlocal Analysis

In this appendix, we will list some results concerning the microlocal analysis of distributions. For a detailed treatment of scalar distributions we refer to [38], whereas Hilbert and Banach-space-valued distributions are treated in [1, 37]. More details concerning distributional sections of vector bundles can be found in, e.g., [1, 16, 34, 41].

Before we discuss distributional sections of vector bundles, we first consider the scaling limit of a distribution in an open set of  $\mathbb{R}^n$ :

**Definition A.1.** Let  $O$  be a convex open region  $O \subset \mathbb{R}^n$  containing 0. For all  $\lambda > 0$  we define the *scaling map*  $\delta_\lambda: O \rightarrow O$  by  $\delta_\lambda(x) := \lambda x$ .

Let  $u$  be a distribution on a convex open region  $O \subset \mathbb{R}^n$  containing 0. The *scaling degree*  $d$  of  $u$  at 0 is defined as  $d := \inf\{\beta \in [-\infty, \infty) \mid \lim_{\lambda \rightarrow 0} \lambda^\beta \delta_\lambda^* u = 0\}$ , where  $(\delta_\lambda^* u)(f) := \lambda^{-n} u(f \circ \delta_\lambda^{-1})$ .

If  $u^0 := \lim_{\lambda \rightarrow 0} \lambda^d \delta_\lambda^* u$  exists we call it the *scaling limit* of  $u$  at 0.

Note that the scaling limit may fail to exist (e.g.,  $u(x) = \log|x|$ ) or it may vanish (e.g., if  $0 \notin \text{supp}(u)$ ). On a manifold, we will only consider scaling limits in a certain choice of local coordinates. How this limit depends on this choice of coordinates will not be relevant for us.

We now prove the following result<sup>w</sup>:

**Proposition A.2.** *Let  $u$  be a distribution on a convex open region  $O \subset \mathbb{R}^n$  containing 0 with scaling limit  $u^0$  at 0. Then*

$$\{0\} \times \pi_2(WF(u^0)) \subset WF(u),$$

where  $\pi_2$  denotes the projection on the second coordinate.

**Proof.** Suppose that  $(0, \xi_0) \notin WF(u)$  with  $\xi_0 \neq 0$ . We will prove that  $(x, \xi_0) \notin WF(u^0)$  for all  $x$ . By assumption, we can choose  $\chi \in C_0^\infty(O)$  and an open conic neighborhood  $\Gamma \subset \mathbb{R}^n$  of  $\xi_0$  such that  $\chi \equiv 1$  on a neighborhood of 0 and  $\text{supp}(\chi) \times \Gamma \cap WF(u) = \emptyset$ . We set  $v := \chi u$  and  $v^\lambda := \lambda^d \delta_\lambda^* v$ , where  $d$  is the scaling degree of  $u$  at 0. Notice that  $WF(v) \cap T_0^* O = WF(u) \cap T_0^* O$  and  $u^0 := \lim_{\lambda \rightarrow 0} v^\lambda$ , so without

<sup>w</sup>A similar result was also claimed as [34, Proposition 2.8], but we find their proof unconvincing. In particular, when localizing the scaling limit  $u^0$  with a test-function  $\chi_0$  and estimating (cf. [34, Eq. (2.11)])

$$\widehat{\chi_0 u^0}(\xi) = \lim_{\lambda \rightarrow 0} \lambda^{d-n} u \left( \chi_0 \left( \frac{\cdot}{\lambda} \right) e^{-i \frac{\xi}{\lambda} \cdot} \right)$$

the test-function  $\chi_0(\frac{\cdot}{\lambda})$  becomes singular in the limit  $\lambda \rightarrow 0$ . The quoted reference pays insufficient attention to this issue in the last sentence of their proof, because their last estimate does not involve any  $\chi_0$ .

loss of generality, we may prove the result with  $v$  replacing  $u$  and we can view the  $v^\lambda$  as compactly supported distributions on all of  $\mathbb{R}^n$ .

Notice that for  $\lambda > 0$  we have  $\delta_\lambda^* u^0 = \lambda^{-d} u^0$ , i.e.  $u^0$  is a homogeneous distribution and therefore it is tempered ([38, Theorem 7.1.18]). We now prove that  $v^\lambda$  converges to  $u^0$  in the sense of tempered distributions on  $\mathbb{R}^n$ . For this we first write  $v = \sum_{|\alpha| \leq r} (-1)^{|\alpha|} \partial^\alpha v_\alpha$ , where  $r$  is the order of  $v$  and the  $v_\alpha$  are compactly supported distributions of order 0 (see [38, Sec. 2.1]). Note that  $\sum_{|\alpha| < d-n} (-1)^{|\alpha|} \partial^\alpha v_\alpha$  converges to 0 in  $\mathcal{S}$ , because for every  $|\alpha| < d-n$  and  $\phi \in \mathcal{S}(\mathbb{R}^n)$  we have

$$|((-1)^{|\alpha|} \partial^\alpha v_\alpha)^\lambda(\phi)| = \lambda^{d-n} |v_\alpha(\partial^\alpha(\phi \circ \delta_\lambda^{-1}))| \leq \lambda^{d-n-|\alpha|} C \sup |\partial^\alpha \phi|$$

which converges to 0 as  $\lambda \rightarrow 0$ . We then set  $w := \sum_{d-n \leq |\alpha| \leq r} (-1)^{|\alpha|} \partial^\alpha v_\alpha$ , so that  $\lim_{\lambda \rightarrow 0} w^\lambda = u^0$  as distributions. By the Uniform Boundedness Principle this implies

$$|w^\lambda(\phi)| \leq C \sum_{|\alpha| \leq r} \sup |\partial^\alpha \phi|, \quad \text{supp}(\phi) \subset B_1, \quad (15)$$

for some  $C, r > 0$ , where  $B_1$  is the (Euclidean) unit ball and  $0 < \lambda \leq 1$ . In fact, for  $\lambda \geq 1$  we also have

$$\begin{aligned} |w^\lambda(\phi)| &= \lambda^{d-n} |w(\phi \circ \delta_\lambda^{-1})| \leq C \sum_{d-n \leq |\alpha| \leq r} \lambda^{d-n-|\alpha|} \sup |\partial^\alpha \phi| \\ &\leq C \sum_{d-n \leq |\alpha| \leq r} \sup |\partial^\alpha \phi|, \end{aligned}$$

so the estimate (15) holds for all  $\lambda > 0$ .

Now, let  $\phi \in \mathcal{S}(\mathbb{R}^n)$  be a function of rapid decrease and choose a partition of unity on  $\mathbb{R}^n$  as follows. We let  $\chi_0 \in C_0^\infty(\mathbb{R}^n)$  be positive such that  $\chi \equiv 1$  on  $B_1$  and  $\chi(x) = 0$  when  $\|x\| \geq 2$ . We then set  $\chi_m(x) := \chi_0(2^{-m}x) - \chi_0(2^{1-m}x)$  and note that:

$$\text{supp}(\chi_{m \geq 1}) \subset \{x \mid 2^{m-1} \leq \|x\| \leq 2^{m+1}\}, \quad \sum_{m=0}^{\infty} \chi_m = 1,$$

where the sum is finite near every point. We define  $\phi_m := \chi_m \phi$  and  $\mu_m := 2^{-m-1}$  and rescale  $\phi_m$  in order to apply the estimate (15):

$$\begin{aligned} |w^\lambda(\phi_m)| &= \mu_m^{d-n} \left| w^{\lambda/\mu_m} \left( \phi_m \left( \frac{\cdot}{\mu_m} \right) \right) \right| \\ &\leq C \sum_{|\alpha| \leq r} \mu_m^{d-n-|\alpha|} \sup \left| (\partial^\alpha \phi_m) \left( \frac{\cdot}{\mu_m} \right) \right| \\ &\leq C_1 \sum_{|\alpha| \leq r} \sum_{|\beta| \leq r+n-d} \sup_{\mathbb{R}^n} |x^\beta \partial^\alpha \phi_m|, \quad m \geq 0, \end{aligned} \quad (16)$$

where the last line uses  $\mu_m^{d-n-|\alpha|} \leq (4\|x\|)^{|\alpha|+n-d}$  for  $m \geq 1$ , which follows from  $d-n \leq |\alpha|$  and the support properties of  $\chi_m$ . (For  $m = 0$  we simply estimate  $\mu_0^{d-n-|\alpha|}$  by a constant to arrive at the last line of (16).) We now note that  $\max_\alpha \sup_x |\partial^\alpha \chi_m| \leq c$  for some  $c$  independent of  $m$ , as the derivatives only bring out extra factors of  $2^{-m} \leq 1$ . Moreover, for  $m \geq 0$  we notice that  $\chi_{m+1} + \chi_m + \chi_{m-1} \equiv 1$  on  $\text{supp}(\chi_m)$ , where we define  $\chi_{-1} := 0$ . Therefore (16) leads to

$$|w^\lambda(\phi_m)| \leq C_2 \sum_{|\alpha| \leq r} \sum_{|\beta| \leq r+n-d} \sup_{\mathbb{R}^n} |x^\beta \partial^\alpha \phi| (\chi_{m+1} + \chi_m + \chi_{m-1})$$

and summing over  $m \geq 0$  then gives:

$$|w^\lambda(\phi)| \leq 3C_2 \sum_{|\alpha| \leq r} \sum_{|\beta| \leq r+n-d} \sup_{\mathbb{R}^n} |x^\beta \partial^\alpha \phi|.$$

This shows that  $w^\lambda(\phi)$  can be estimated by a seminorm on  $\mathcal{S}(\mathbb{R}^n)$  uniformly in  $\lambda$ . It then follows that  $w^\lambda \rightarrow u^0$  and hence  $v^\lambda \rightarrow u^0$  as tempered distributions. Indeed, for any  $\phi \in \mathcal{S}(\mathbb{R}^n)$  and  $\epsilon > 0$  we can choose  $\phi' \in C_0^\infty(\mathbb{R}^n)$  and  $\lambda_0 > 0$  such that  $|w^\lambda(\phi - \phi')| < \frac{\epsilon}{2}$  for all  $\lambda > 0$  and  $|w^\lambda(\phi')| < \frac{\epsilon}{2}$  for all  $\lambda < \lambda_0$ .

Fourier transformation is a continuous operation on tempered distributions, so we can compute:

$$|\widehat{u^0}(\xi)| = \lim_{\lambda \rightarrow 0} \lambda^{d-n} \left| \widehat{v} \left( \frac{\xi}{\lambda} \right) \right| \leq C_N \lim_{\lambda \rightarrow 0} \lambda^{d-n} \left\| \frac{\xi}{\lambda} \right\|^{-N} = C_N \|\xi\|^{-N} \lim_{\lambda \rightarrow 0} \lambda^{N+d-n}$$

for all  $\xi$  in  $\Gamma$ , all  $N \in \mathbb{N}$  and suitable  $C_N > 0$ . For  $N > n-d$  the limit yields  $\widehat{u^0}(\xi) = 0$  near  $\xi_0$ . We then apply [38, Theorem 8.1.8], which says that for a homogeneous distribution we have for all  $x \neq 0$  that  $(x, \xi_0) \in WF(u^0)$  if and only if  $(\xi_0, -x) \in WF(\widehat{u^0})$  and also  $(0, \xi_0) \in WF(u^0)$  if and only if  $\xi_0 \in \text{supp}(\widehat{u^0})$ .  $\square$

For a distribution  $u$  with values in a Banach space  $\mathcal{B}$  one can define the wave front set by using estimates of the norm  $\|u(\chi e^{i\xi \cdot})\|$ , which replace the corresponding estimates of the absolute value  $|u(\chi e^{i\xi \cdot})|$  for scalar distributions [37]. Alternatively, one can use the following equivalent characterization ([1, Theorem A.1.4]):

$$WF(u) = \overline{\bigcup_{l \in \mathcal{B}'} WF(l \circ u) \setminus \mathcal{Z}}. \quad (17)$$

A similar idea works for a distributional section  $u$  of a vector bundle  $\mathcal{V} = O \times \mathbb{R}^m$  over a contractible region  $O$  of  $\mathbb{R}^n$ . Indeed, using a basis  $e_i$  for  $\mathbb{R}^m$  with dual basis  $e^i$  we can identify  $u$  with a distribution  $\tilde{u}$  on  $O$  with values in  $\mathcal{B} \otimes (\mathbb{R}^m)'$ , where the correspondence is given by

$$\tilde{u}(h) := \sum_{i=1}^m u(h e_i) \otimes e^i, \quad u \left( \sum_{i=1}^m f^i e_i \right) = \sum_{i=1}^m \langle \tilde{u}(f^i), e_i \rangle,$$



where  $\langle \cdot, \cdot \rangle$  denotes the canonical pairing of  $\mathbb{R}^m$  with the second factor of  $\mathcal{B} \otimes (\mathbb{R}^m)'$ . We set by definition  $WF(u) := WF(\tilde{u})$ .

Equation (17) allows a straightforward generalization of many results for scalar distributions on open sets of  $\mathbb{R}^n$  to Banach-space-valued distributional sections of a vector bundle over regions over  $\mathbb{R}^n$ . Moreover, by showing how these results transform under changes of coordinates they can be formulated for vector bundles on a manifold. We list a number of these results in the following Theorem (cf. [1, 38]):

**Theorem A.3.** *If  $u, v$  are distributional sections of a complex vector bundle  $\mathcal{V}$  over the spacetime  $M$  with values in the Banach space  $\mathcal{B}$ , then:*

- (1) *sing supp( $u$ ) is the projection of  $WF(u)$  on the first variable,*
- (2)  *$u \in C^\infty(\mathcal{V}, \mathcal{B})$  if and only if  $WF(u) = \emptyset$ ,*
- (3)  *$WF(u + v) \subset WF(u) + WF(v)$ ,*
- (4) *if  $P$  is a linear partial differential operator on  $\mathcal{V}$  with smooth coefficients and (matrix-valued) principal symbol<sup>\*</sup>  $p(x; \xi)$ , then  $WF(Pu) \subset WF(u) \subset WF(Pu) \cup \Omega_P$ , where  $\Omega_P := \{(x; \xi) \in T^*M \mid \xi \neq 0, \det p(x; \xi) = 0\}$ ,*
- (5) *if  $x \in M$ ,  $\phi: U \rightarrow \mathbb{R}^n$  is a local trivialization on a convex neighborhood  $U$  with  $\phi(x) = 0$  and  $(\phi^{-1})^*u$  has a scaling limit  $u^0$  at 0, then  $\phi^*(\{0\} \times \pi_2(WF(u^0))) \subset WF(u) \cap T_x^*M$ .*

In the last item, the scaling limit depends not just on the choice of coordinates, but also on the choice of a frame  $e_i$  of  $\mathcal{V}$  over  $U$  and we let the scaling maps  $\delta_\lambda$  act on sections of  $\mathcal{V}$  componentwise:  $(\sum_i f^i e_i) \circ \delta_\lambda^{-1} = \sum_i (f^i \circ \delta_\lambda^{-1}) e_i$ .

In the particular case where  $\mathcal{B}$  is a Hilbert space, we also have (see [1, 37]):

**Theorem A.4.** *Let  $\mathcal{H}$  be a Hilbert space and  $\mathcal{V}_i, i = 1, 2$ , two finite-dimensional (complex) vector bundles over smooth  $n_i$  dimensional spacetimes  $M_i$  with complex conjugations  $J_i$ , i.e. the  $J_i$  are antilinear, base-point preserving bundle isomorphisms  $J_i: \mathcal{V}_i \rightarrow \mathcal{V}_i$  such that  $J_i^2 = -id$ . Let  $u_i, i = 1, 2$ , be two  $\mathcal{H}$ -valued distributional sections of  $\mathcal{V}_i$  and let  $w_{ij}$  be the distributional sections of the vector bundle  $\mathcal{X}_i \boxtimes \mathcal{X}_j$  over  $M_i \times M_j$  determined by  $w_{ij}(f_1 \boxtimes f_2) := \langle u_i(J_i f_1), u_j(f_2) \rangle$ . Then*

$$(x, \xi) \in WF(u_1) \Leftrightarrow (x, -\xi; x, \xi) \in WF(w_{11})$$

and

$$WF(w_{ij}) \subset -(WF(u_i) \cup \mathcal{Z}) \times (WF(u_j) \cup \mathcal{Z}),$$

where  $\mathcal{Z}$  denotes the zero-section.

Finally, we establish some results on the wave front sets of advanced and retarded fundamental solutions  $E^\pm$  (for their existence and uniqueness we refer to [16]) and  $S^\pm, S_c^\pm$ . These results are analogous to [36, Theorem 6.5.3], but now

<sup>\*</sup>See [16] for the definition of the principal symbol.

for operators in a vector bundle. Note that for distributional sections of vector bundles there is a Propagation of Singularities Theorem, which follows from the propagation of the polarization set [41].

**Theorem A.5.** *Let  $E^\pm$  be the advanced  $(-)$  and retarded  $(+)$  fundamental solutions for a normally hyperbolic operator  $P$  acting on the sections of a vector bundle  $DM$  over a globally hyperbolic spacetime  $M = (\mathcal{M}, g)$  of dimension  $n \geq 2$ . Then*

$$\begin{aligned} WF(E^\pm) &= \{(x, \xi; y, \eta) \in T^*M^{\times 2} \setminus \mathcal{Z} \mid x \in J^\pm(y), x \neq y, (x, -\xi) \sim (y, \eta)\} \\ &\quad \cup \{(x, -\xi; x, \xi) \in T^*M^{\times 2} \setminus \mathcal{Z} \mid (x, \xi) \in T^*M \setminus \mathcal{Z}\} \\ &=: A^\pm \cup B \end{aligned} \tag{18}$$

where  $\mathcal{Z}$  is the zero-section and  $(x, \xi) \sim (y, \eta)$  if and only if there is a light-like geodesic  $\gamma$  from  $x$  to  $y$  to which  $\xi$  and  $\eta$  are cotangent such that they are each others parallel transport along  $\gamma$ .

**Proof.** The first part of this proof follows closely the proof of [31].

We start by reducing the problem to a local one as follows. The principal symbol of  $P$  is  $p(x, \xi) = g_{\mu\nu}(x)\xi^\mu\xi^\nu I$ , where  $I$  is the identity operator on  $DM$ , so by the Propagation of Singularities Theorem, the singularities of  $E^\pm$  propagate along light-like geodesics by parallel transport. By definition the points in set  $A^\pm$  are invariant under the same parallel transport. Now consider a point  $p := (x, \xi; y, \eta)$  with  $x \neq y$ . If  $\xi = \eta = 0$  then  $P$  is not contained in any set on either side of the equality, so we may assume  $\xi \neq 0$  (the case  $\eta \neq 0$  is analogous). Let  $S$  be a spacelike Cauchy surface through  $y$  and propagate  $(x, \xi)$  along the light-like geodesic  $\gamma$  towards  $S$ . If  $\gamma$  ends at  $S$  in  $x' \neq y$  then  $P$  is not contained in  $A^\pm$  or  $B$ , nor is it contained in  $WF(E^\pm)$ , because  $E(x', y) = 0$  when  $x'$  and  $y$  are spacelike, so it cannot have any singularities there. If  $\gamma$  ends at  $y$ , on the other hand, we can find a point  $p' := (x', \xi'; y, \eta)$ , where  $x'$  on  $\gamma$  is in any given causally convex neighborhood of  $y$  and  $\xi'$  is the parallel transport of  $\xi$  along  $\gamma$  to  $x'$ . Then  $p' \in WF(E^\pm)$  if and only if  $p \in WF(E^\pm)$  and  $p' \in A^\pm$  if and only if  $p \in A^\pm$ . Hence, it suffices to prove the claim locally.

On a sufficiently small causally convex domain  $O \subset \mathcal{M}$  we can find for every  $k \in \mathbb{N}$  a  $C^k$ -section  $W^k$  of  $DM \boxtimes D^*M$  on  $O^{\times 2}$  such that ([16, Proposition 2.5.1]):

$$E^\pm(x, y) = \sum_{j=0}^{k+1} V_j(x, y) f^*(1 \otimes R^\pm(2 + 2j, \cdot))(x, y) + W^k(x, y). \tag{19}$$

Here, the Hadamard coefficients  $V_j$  are uniquely defined smooth sections of  $DM \boxtimes D^*M$  on  $O^{\times 2}$ ,  $R^\pm(\alpha, y)$  are the retarded  $(+)$  and advanced  $(-)$  Riesz distributions (or rather distribution densities) on Minkowski spacetime and they are pulled back by the smooth diffeomorphism  $f: O^{\times 2} \rightarrow TO$  defined by  $(x, y) \mapsto (x, \exp_x^{-1}(y))$ . This means we use Riemannian normal coordinates for  $y$  centered on  $x$ , which is

well-defined because  $O$  is causally convex. The Riesz distributions have many useful properties, of which we will only use for all  $j \geq 0$ :

$$\begin{aligned} WF(R^\pm(2j+2, \cdot)) &= \{(x, \xi) \in T^*M_0 \setminus \mathcal{Z} \mid x = 0 \text{ or } x^2 = 0, x \in J^\pm(0), \xi \parallel x\} \\ R^\pm(2+2j, \lambda x) &= \lambda^{2+2j-n} R^\pm(2+2j, x), \quad \lambda > 0. \end{aligned} \tag{20}$$

(These can be proved using [16, Proposition 1.2.4 items 4 and 5],  $\square^{j+1}R^\pm(2+2j, \cdot) = \delta$  and the wave front sets of the distinguished parametrices as determined in [36].) Hence, for all  $j \in \mathbb{N}$ :

$$\begin{aligned} WF(f^*(1 \otimes R^\pm(2+2j, \cdot))) &= f^*(WF(1 \otimes R^\pm(2+2j, \cdot))) \\ &= f^*(\mathcal{Z}|_O \times WF(R^\pm(2+2j, \cdot))) \\ &= \{(x, \xi; y, \eta) \mid (\xi, \eta) = df^T(0, \eta') \text{ for some} \\ &\quad (\exp_x^{-1}(y), \eta') \in WF(R^\pm(2+2j, \cdot))\}, \\ &= (A^\pm \cup B) \cap T^*O^{\times 2}, \end{aligned} \tag{21}$$

where  $df^T$  is the transpose of the derivative  $df$  at  $(x, y)$ . The last equality uses the wave front set of the Riesz distributions in Eq. (20) and the properties of Riemannian normal coordinates (cf. [31]). It follows that  $WF(E^\pm|_{O^{\times 2}}) \subset (A^\pm \cup B) \cap T^*O^{\times 2}$ , because for each order of differentiation  $N$  we can choose a sufficiently high order  $k$  in Eq. (19) to make the required estimate in the definition of the wave front set.

We can prove the opposite inclusion, if we can show that the wave front set of the finite sum in (19) also contains  $(A^\pm \cup B) \cap T^*O^{\times 2}$ , which we will do using scaling limits (cf. [34]). First, we may employ the Riemannian normal coordinates  $f: O^{\times 2} \rightarrow TO$  as above. Next, we may assume that  $O$  is also a contractible coordinate neighbourhood, so we can consider local coordinates  $\phi: O \rightarrow \mathbb{R}^n$  on  $O$  and the associated coordinate map  $d\phi$  on  $TO$ . Moreover, we can choose  $\phi$  in such a way that  $\phi(x_0) = 0$  for an arbitrarily given  $x_0 \in O$ . The composition  $d\phi \circ f$  then defines coordinates on  $O^{\times 2}$  such that  $(x_0, x_0) \mapsto 0 \in \mathbb{R}^{2n}$ . Using a frame  $E_A$  for  $DM|_O$  and the dual frame  $E^B$  we can express the terms in the sum of Eq. (19) in the local coordinates  $d\phi \circ f$  as  $V_{jB}^A(x, y)R^\pm(2+2j, y)$ . From Eq. (20), we then find the scaling behavior

$$\delta_\lambda^*(V_{jB}^A(x, y)R^\pm(2+2j, y)) = \lambda^{2+2j-n}(V_{jB}^A(\lambda x, \lambda y)R^\pm(2+2j, y))$$

for all  $\lambda > 0$ . In the scaling limit only the lowest order term survives:

$$\begin{aligned} \lim_{\lambda \rightarrow 0} \lambda^{n-2}(\delta_\lambda \circ f^{-1} \circ d\phi^{-1})^* E(x, y) &= V_{0B}^A(0, 0)R(2, y)E^B(x)E_A(y) \\ &= R(2, y)E^A(x)E_A(y), \end{aligned}$$

where we wrote  $R(2, y) := R^-(2, y) - R^+(2, y)$  and we used the explicit expression  $V_{0B}^A(x, x) = \delta_B^A$  ([16, Lemmas 2.2.2 and 1.3.17]).

Now, the last item of Theorem A.3 (which follows from Proposition A.2) implies that  $WF(E) \supset (d\phi \circ f)^*(\{(0, 0)\} \times \pi_2(WF(1 \otimes R(2, \cdot))))$ , because  $E^A(x)E_A(y)$  is smooth and not identically vanishing. From Eq. (20) and the support properties of  $R^\pm(2, \cdot)$  we easily compute  $\pi_2(WF(1 \otimes R(2, \cdot))) = \{(0, \xi) \mid \xi^2 = 0\}$ . Pulling this back to  $O^{\times 2}$  and using the properties of Riemannian normal coordinates yields

$$WF(E) \supset \{(x_0, -\xi; x_0, \xi) \mid \xi^2 = 0\}.$$

Because  $E$  is a bi-solution to the wave equation we can apply the Propagation of Singularities Theorem to find that  $WF(E) \supset A^+ \cup A^-$  on  $O^{\times 2}$  and from the support properties of  $E^+$  and  $E^-$  we then conclude that  $WF(E^\pm) \supset A^\pm$ . Finally,  $WF(E^\pm) \supset WF(PE^\pm) = WF(\delta) = B$ . This completes the proof.  $\square$

**Corollary A.6.** *In the notation of Theorem A.5,  $WF(E) = \overline{A^+ \cup A^-} \setminus \mathcal{Z}$ .*

**Proof.** By Theorem A.5 and the support properties of  $E^\pm$ , we have  $WF(E) = A^+ \cup A^-$  away from the diagonal. The inclusion  $\supset$  then follows from the closedness of the wave front set. For the opposite inclusion we consider a point on the diagonal and use the Propagation of Singularities Theorem to find an approximating sequence of points off the diagonal.  $\square$

**Proposition A.7.** *For the fundamental solutions of the Dirac equation we have, in the notation of Theorem A.5:  $WF(S^\pm) = WF(S_c^\pm) = A^\pm \cup B$  and  $WF(S) = WF(S_c) = \overline{A^+ \cup A^-} \setminus \mathcal{Z}$ .*

In other words,  $WF(S^\pm) = WF(S_c^\pm) = WF(E^\pm)$  and  $WF(S) = WF(S_c) = WF(E)$ .

**Proof.** Because  $S^\pm = (i\nabla + m)E^\pm$  and  $S_c^\pm = (-i\nabla + m)E^\pm$  (see [6]) we immediately find  $WF(S^\pm) \subset WF(E^\pm)$  and  $WF(S_c^\pm) \subset WF(E^\pm)$ . Similarly  $WF(S) \subset WF(E)$  and  $WF(S_c) \subset WF(E)$ . Now suppose that  $WF(S) = WF(S_c) = WF(E) = \overline{A^+ \cup A^-}$ , which we will prove below. By the support properties of the fundamental solutions we then find that away from the diagonal  $WF(S^\pm) = WF(S_c^\pm) = A^\pm$ , whereas on the diagonal  $WF(E^\pm) = B \supset WF(S^\pm) \supset WF(PS^\pm) = WF(\delta) = B$  and similarly for cospinors.

To complete the proof we need to show that  $WF(S) \supset WF(E)$  and  $WF(S_c) \supset WF(E)$ , for which we adapt (and correct) an idea of [33]. We prove the case of  $S$ , because the other case follows by taking adjoints (cf. Theorem 3.10). Further note that it is sufficient to prove the claim on the diagonal, because the Propagation of Singularities Theorem applies both to  $E$  and to  $S$ . Now suppose that  $(x, -\xi; x, \xi) \in WF(E) \setminus WF(S)$ . We will derive a contradiction as follows. For every time-like, future pointing normalized vector  $n_0 \in T_x M$  we can find a smooth space-like Cauchy surface  $C$  through  $x$  such that  $n_0$  is normal to  $C$ . We let  $n$  denote

the future pointing normal vector field on  $C$  and  $\iota: C \rightarrow M$  the canonical injection. By [6, Proposition 2.4(c)] we can restrict  $S$  to  $C^{\times 2}$  to find  $S|_{C^{\times 2}} = -i\delta\eta$  and in particular  $(x, -d\iota_x^T(\xi); x, d\iota_x^T(\xi)) \in WF(S|_{C^{\times 2}})$ . By (a component version of) [38, Theorem 8.2.4], on the other hand:

$$WF(S|_{C^{\times 2}}) \subset (\iota \times \iota)^*(WF(S)) = \{(x, d\iota_x^T(\xi); y, d\iota_y^T(\xi')) \mid (x, \xi; y, \xi') \in WF(S)\}.$$

Therefore, there must be a point  $(x, -\eta; x, \eta) \in WF(S)$  such that  $(x, -d\iota_x^T(\eta); x, d\iota_x^T(\eta)) = (x, -d\iota_x^T(\xi); x, d\iota_x^T(\xi))$ . Notice, however, that the transpose of  $d\iota$  is nothing else than restricting the dual vector  $\xi$  to the tangent space of  $C$ . Because  $WF(S) \subset WF(E)$ , there are only two possibilities:  $\eta = \xi$  or  $\eta = \xi - 2(\xi_a n_0^a) n_0$ . The first contradicts our assumption, so we have  $\eta = \xi - 2(\xi_a n_0^a) n_0$ . Now  $(x, -\eta; x, \eta) \in WF(S)$  must hold for every normalised, time-like, future pointing vector  $n_0 \in T_x M$ . Choosing a sequence of vectors  $n_0$  such that  $\eta \rightarrow \xi$  and using the closedness of the wave front set we find again  $(x, -\xi; x, \xi) \in WF(S)$ . Hence,  $WF(E) = WF(S)$ .  $\square$

## Appendix B. Proof of Theorem 4.18

The computations involved in the proof of Theorem 4.18 are somewhat similar to the computation of the stress-energy-momentum tensor. We will work in components and in local coordinates on  $O$ , using Greek indices to indicate the coordinate frame and coordinate derivatives. To ease the notation we will drop the subscript  $\epsilon$  on the local frame  $e_a^\mu$ .

As  $\gamma^a$  is independent of  $\epsilon$  we may use Eqs. (5) to vary

$$\nabla v = \left( \partial_a v - \frac{1}{4} \Gamma_{ab}^c v \gamma_c \gamma^b \right) \gamma^a = e_a^\alpha \left( \partial_\alpha v + \frac{1}{4} e_b^\beta \{ \partial_\alpha e_\beta^c - e_\gamma^c \Gamma_{\alpha\beta}^\gamma \} v \gamma_c \gamma^b \right) \gamma^a, \quad (22)$$

which yields:

$$\begin{aligned} \delta \nabla v &= \delta e_a^\alpha e_\alpha^d \nabla_d v \gamma^a - \frac{1}{4} \delta e_b^\beta e_\beta^d \Gamma_{ad}^c v \gamma_c \gamma^b \gamma^a + \frac{1}{4} \partial_a \delta e_\beta^c e_b^\beta v \gamma_c \gamma^b \gamma^a \\ &\quad - \frac{1}{4} \delta e_\gamma^c e_a^\alpha e_b^\beta \Gamma_{\alpha\beta}^\gamma v \gamma_c \gamma^b \gamma^a - \frac{1}{4} \delta \Gamma_{\alpha\beta}^\gamma e_a^\alpha e_b^\beta e_\gamma^c v \gamma_c \gamma^b \gamma^a. \end{aligned} \quad (23)$$

We can perform an integration by parts as follows:

$$\begin{aligned} &\frac{1}{4} \partial_a \delta e_\beta^c e_b^\beta v \gamma_c \gamma^b \gamma^a \\ &= \frac{-i}{4} P_c (\delta e_\beta^c e_b^\beta v \gamma_c \gamma^b) + \frac{i}{4} \delta e_\beta^c e_b^\beta P_c (v \gamma_c \gamma^b) \\ &\quad - \frac{1}{4} \delta e_\beta^c \partial_a e_b^\beta v \gamma_c \gamma^b \gamma^a - \frac{1}{4} \delta e_\beta^d e_b^\beta \Gamma_{ad}^c v \gamma_c \gamma^b \gamma^a + \frac{1}{4} \delta e_\beta^c e_d^\beta \Gamma_{ab}^d v \gamma_c \gamma^b \gamma^a \end{aligned}$$

$$\begin{aligned}
&= -\frac{i}{4}P_c(\delta e_\beta^c e_b^\beta v\gamma_c\gamma^b) + \frac{i}{4}\delta e_\beta^c e_b^\beta (P_c v)\gamma_c\gamma^b - \frac{1}{4}\delta e_\beta^c e_b^\beta \nabla_a v[\gamma_c\gamma^b, \gamma^a] \\
&\quad - \frac{1}{4}\delta e_\beta^c \partial_a e_b^\beta v\gamma_c\gamma^b\gamma^a + \frac{1}{4}\delta e_b^\beta e_\beta^d \Gamma_{ad}^c v\gamma_c\gamma^b\gamma^a + \frac{1}{4}\delta e_\beta^c e_d^\beta \Gamma_{ab}^d v\gamma_c\gamma^b\gamma^a.
\end{aligned} \tag{24}$$

Because  $[\gamma_c\gamma^b, \gamma^a] = \gamma_c\{\gamma^b, \gamma^a\} - \{\gamma_c, \gamma^a\}\gamma^b = 2\eta^{ab}\gamma_c - 2\delta_c^a\gamma^b$  and  $e_\beta^c = g_{\mu\beta}\eta^{cd}e_d^\mu$  we can write:

$$\begin{aligned}
-\frac{1}{4}\delta e_\beta^c e_b^\beta \nabla_a v[\gamma_c\gamma^b, \gamma^a] &= -\frac{1}{2}\delta(g_{\mu\beta}\eta^{cd}e_d^\mu)e_b^\beta\eta^{ab}\nabla_a v\gamma_c + \frac{1}{2}\delta e_\beta^c e_b^\beta \nabla_c v\gamma^b \\
&= -\frac{1}{2}\delta g_{\mu\beta}\eta^{cd}e_d^\mu e_b^\beta\eta^{ab}\nabla_a v\gamma_c - \delta e_d^\mu e_\mu^a \nabla_a v\gamma^d \\
&= \frac{1}{2}\delta g^{\alpha\beta}e_\alpha^a e_\beta^b \nabla_a v\gamma_b - \delta e_\alpha^a e_\alpha^d \nabla_d v\gamma^a.
\end{aligned} \tag{25}$$

When substituting Eqs. (24) and (25) into (23), we can recombine the terms

$$-\frac{1}{4}\delta e_\beta^c \partial_a e_b^\beta v\gamma_c\gamma^b\gamma^a - \frac{1}{4}\delta e_\gamma^c e_\alpha^a e_b^\beta \Gamma_{\alpha\beta}^\gamma v\gamma_c\gamma^b\gamma^a = -\frac{1}{4}\delta e_\gamma^c e_d^\beta \Gamma_{ab}^d v\gamma_c\gamma^b\gamma^a$$

to obtain

$$\begin{aligned}
\delta\mathcal{V}v &= \frac{-i}{4}P_c(\delta e_\beta^c e_b^\beta v\gamma_c\gamma^b) + \frac{i}{4}\delta e_\beta^c e_b^\beta (P_c v)\gamma_c\gamma^b + \frac{1}{2}\delta g^{\alpha\beta}e_\alpha^a e_\beta^b \nabla_a v\gamma_b \\
&\quad - \frac{1}{4}\delta \Gamma_{\alpha\beta}^\gamma e_\alpha^a e_\beta^b e_\gamma^c v\gamma_c\gamma^b\gamma^a.
\end{aligned} \tag{26}$$

Note that the variations of the frame  $\delta e_a^\alpha$  cancel out, except in the terms with  $P_c$ . These are harmless when we compute  $B_0(\delta\mathcal{V}S_0f)$ , because both  $B_0$  and  $v$  solve the Dirac equation. Therefore, the final answer will not depend on variations of the frame, as desired.

In the last term of Eq. (26), we can use the symmetry of the Christoffel symbol:

$$\begin{aligned}
-\frac{1}{4}\delta \Gamma_{(\alpha\beta)}^\gamma e_\alpha^a e_\beta^b e_\gamma^c v\gamma_c\gamma^b\gamma^a &= -\frac{1}{4}\delta \Gamma_{\alpha\beta}^\gamma e_\alpha^a e_\beta^b e_\gamma^c v\gamma_c\eta^{ab} = -\frac{1}{4}\delta \Gamma_{\alpha\beta}^\gamma g^{\alpha\beta} e_\gamma^c v\gamma_c \\
&= -\frac{1}{4}\delta g^{\gamma\mu}g_{\mu\nu}\Gamma_{\alpha\beta}^\nu e_\gamma^c v\gamma_c - \frac{1}{4}\partial_\alpha \delta g_{\beta\mu}e_\alpha^\mu g^{\alpha\beta} v\gamma^a \\
&\quad + \frac{1}{8}\partial_\mu \delta g_{\alpha\beta}e_\alpha^\mu g^{\alpha\beta} v\gamma^a.
\end{aligned} \tag{27}$$

We handle the last term using an integration by parts as before:

$$\begin{aligned}
\frac{1}{8}\partial_a \delta g_{\alpha\beta}g^{\alpha\beta} v\gamma^a &= \frac{-i}{8}P_c(\delta g_{\alpha\beta}g^{\alpha\beta}v) + \frac{i}{8}\delta g_{\alpha\beta}g^{\alpha\beta}P_c v - \frac{1}{8}\delta g_{\alpha\beta}\partial_a g^{\alpha\beta}v\gamma^a \\
&= \frac{-i}{8}P_c(\delta g_{\alpha\beta}g^{\alpha\beta}v) + \frac{i}{8}\delta g_{\alpha\beta}g^{\alpha\beta}P_c v - \frac{1}{8}\delta g^{\alpha\beta}\partial_a g_{\alpha\beta}v\gamma^a, \tag{28}
\end{aligned}$$

where we used  $\delta g_{\alpha\beta} \partial_a g^{\alpha\beta} = -\delta g^{\alpha\beta} g_{\alpha\mu} g_{\beta\nu} \partial_a g^{\mu\nu} = \delta g^{\alpha\beta} \partial_a g_{\alpha\beta}$ . The penultimate term in (27) is:

$$\begin{aligned}
-\frac{1}{4} \partial_\alpha \delta g_{\beta\mu} e_a^\mu g^{\alpha\beta} v \gamma^a &= \frac{1}{4} \partial_b (\delta g^{\alpha\beta} g_{\alpha\mu} g_{\beta\nu}) e_a^\mu e_\rho^b g^{\rho\nu} v \gamma^a \\
&= \frac{1}{4} \partial_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b) v \gamma_a - \frac{1}{4} \delta g^{\alpha\beta} g_{\alpha\mu} g_{\beta\nu} \partial_b (e_a^\mu e_\rho^b g^{\rho\nu}) v \gamma^a \\
&= \frac{1}{4} \nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b) v \gamma_a - \frac{1}{4} \delta g^{\alpha\beta} (\Gamma_{bc}^a e_\alpha^c e_\beta^b + \Gamma_{bc}^b e_\alpha^a e_\beta^c) v \gamma_a \\
&\quad - \frac{1}{4} \delta g^{\alpha\beta} g_{\alpha\mu} g_{\beta\nu} \partial_b (e_a^\mu e_\rho^b g^{\rho\nu}) v \gamma^a.
\end{aligned} \tag{29}$$

The first term on the right-hand side of Eq. (29) is

$$\frac{1}{4} \nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b) v \gamma_a = \frac{1}{4} \nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b v \gamma_a) - \frac{1}{4} \delta g^{\alpha\beta} e_\alpha^a e_\beta^b \nabla_b v \gamma_a. \tag{30}$$

The other terms can be simplified with some computation:

$$\begin{aligned}
&-\frac{1}{4} \delta g^{\alpha\beta} (\Gamma_{bc}^a e_\alpha^c e_\beta^b + \Gamma_{bc}^b e_\alpha^a e_\beta^c + g_{\alpha\mu} g_{\beta\nu} \eta^{ac} \partial_b (e_c^\mu e_\rho^b g^{\rho\nu})) v \gamma_a \\
&= -\frac{1}{4} \delta g^{\alpha\beta} (-\partial_\beta e_\alpha^a + e_\gamma^a \Gamma_{\beta\alpha}^\gamma - e_\alpha^a \partial_c e_\beta^c + e_\alpha^a \Gamma_{\mu\beta}^\mu) \\
&\quad + e_\alpha^a g_{\beta\nu} \partial_\rho g^{\rho\nu} + e_\alpha^a \partial_b e_\beta^b + g_{\alpha\mu} \eta^{ac} \partial_\beta e_c^\mu) v \gamma_a \\
&= -\frac{1}{4} \delta g^{\alpha\beta} (-\eta^{ac} e_c^\mu \partial_\beta g_{\alpha\mu} + e_\gamma^a \Gamma_{\beta\alpha}^\gamma + e_\alpha^a \Gamma_{\mu\beta}^\mu - e_\alpha^a g^{\rho\nu} \partial_\rho g_{\beta\nu}) v \gamma_a \\
&= -\frac{1}{8} \delta g^{\alpha\beta} (-2e_\gamma^a g^{\gamma\mu} \partial_\beta g_{\alpha\mu} + e_\gamma^a g^{\gamma\mu} (2\partial_\beta g_{\alpha\mu} - \partial_\mu g_{\alpha\beta})) \\
&\quad + e_\alpha^a g^{\mu\gamma} \partial_\beta g_{\mu\gamma} - 2e_\alpha^a g^{\rho\nu} \partial_\rho g_{\beta\nu}) v \gamma_a \\
&= \frac{1}{8} \delta g^{\alpha\beta} (e_\gamma^a g^{\gamma\mu} \partial_\mu g_{\alpha\beta} + 2e_\alpha^a g_{\beta\mu} g^{\rho\nu} \Gamma_{\rho\nu}^\mu) v \gamma_a.
\end{aligned} \tag{31}$$

Substituting Eqs. (27)–(31) into (26) yields:

$$\begin{aligned}
\delta \nabla v &= \frac{-i}{4} P_c (\delta e_\beta^c e_b^\beta v \gamma_c \gamma^b) + \frac{i}{4} \delta e_\beta^c e_b^\beta (P_c v) \gamma_c \gamma^b - \frac{i}{8} P_c (\delta g_{\alpha\beta} g^{\alpha\beta} v) + \frac{i}{8} \delta g_{\alpha\beta} g^{\alpha\beta} P_c v \\
&\quad + \frac{1}{4} \delta g^{\alpha\beta} e_\alpha^a e_\beta^b \nabla_a v \gamma_b + \frac{1}{4} \nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b v \gamma_a).
\end{aligned} \tag{32}$$

Using Lemma 4.17, we find for a spinor  $u \in C^\infty(DM)$ :

$$\begin{aligned} \delta \nabla u &= \frac{i}{4} P(\delta e_\beta^c e_b^\beta \gamma^b \gamma_c u) - \frac{i}{4} \delta e_\beta^c e_b^\beta \gamma^b \gamma_c (Pu) + \frac{i}{8} P(\delta g_{\alpha\beta} g^{\alpha\beta} u) - \frac{i}{8} \delta g_{\alpha\beta} g^{\alpha\beta} Pu \\ &\quad + \frac{1}{4} \delta g^{\alpha\beta} e_\alpha^a e_\beta^b \gamma_b \nabla_a u + \frac{1}{4} \nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b \gamma_a u). \end{aligned} \quad (33)$$

Using Proposition 4.16 and Eqs. (32) and (33) we notice that the terms with  $P_c$  and  $P$  cancel out in the following equality, because  $B_0$  and  $S_0 f$  both satisfy the Dirac equation:

$$\begin{aligned} \delta(\beta_\epsilon B_0(f)) &= -B_0(\delta P_\epsilon S_0 f) \\ &= \frac{i}{4} B_0(\delta g^{\alpha\beta} e_\alpha^a e_\beta^b \gamma_b \nabla_a S_0 \tau f) + \frac{i}{4} B_0(\nabla_b (\delta g^{\alpha\beta} e_\alpha^a e_\beta^b \gamma_a S_0 \tau f)) \\ &= \frac{i}{4} \delta g^{\alpha\beta} e_\alpha^a e_\beta^b (B_0(\gamma_{(b} \nabla_a) S_0 \tau f) - \nabla_{(b} B_0(\gamma_a) S_0 \tau f)). \end{aligned} \quad (34)$$

We now compare with Proposition 4.14 to get the final result.

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